Low-temperature anomalies in glasses from the mean-field viewpoint

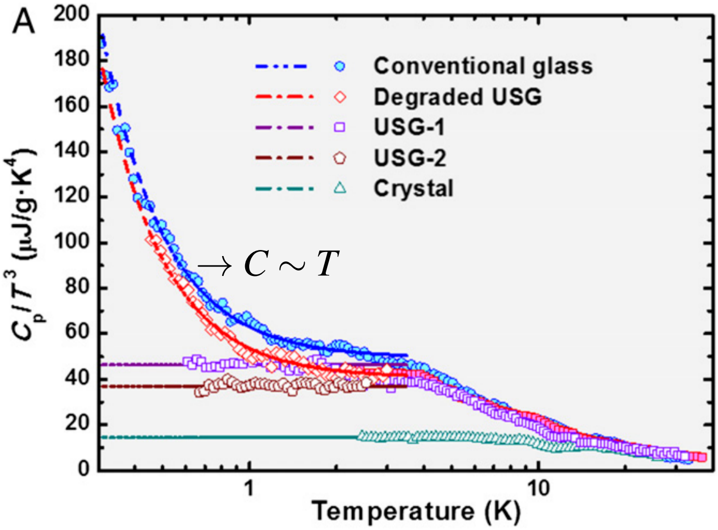
Thibaud Maimbourg

References:

Franz, Maimbourg, Parisi, Scardicchio *PNAS* 2019 *(jamming transition)*

Maimbourg, Urbani *[in preparation]*

Anomalous scalings in glasses at very low temperature



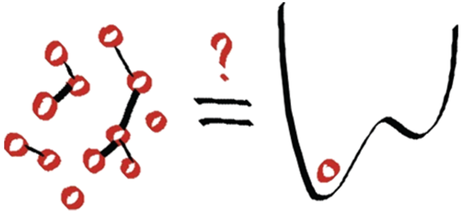
[Zeller, Pohl *PRB* 1971]
[Pérez-Castañeda, Rodríguez-Tinoco, Rodríguez-Viejo, Ramos *PNAS* 2014]

Debye: $H \approx E_{\min} + \frac{1}{2}\sum_i m_i \omega_i^2 x_i^2$ with acoustic phonons $\omega \propto k \Rightarrow C \sim T^d$

Tunneling two-level systems (TTLS) and phenomenology

Standard Tunneling Model

[Anderson Halperin Varma *Phil. Mag.* 1972] [Phillips *J. Low. Temp. Phys.* 1972]

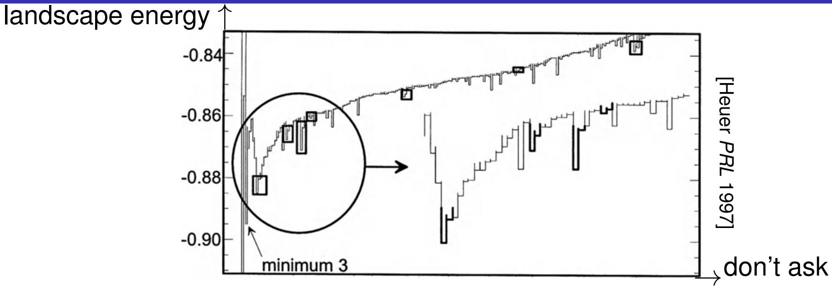


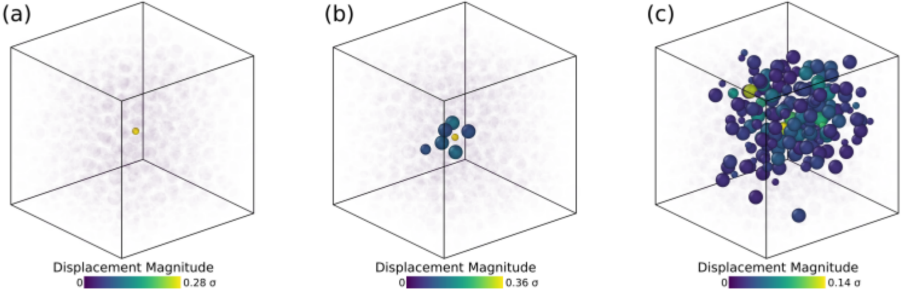
assume flat DOS $\rho(\varepsilon) \to \rho(0) \neq 0$

$$C_V = \frac{\partial}{\partial T} \int_0^\infty \mathrm{d}\varepsilon\, \rho(\varepsilon) \frac{\varepsilon}{e^{\beta\varepsilon}+1} \underset{T\to 0}{\propto} \rho(0) T$$

- **Soft Potential Model (1980s):** low-energy modes given by *independent* oscillators $v(x) \propto hx + mx^2 + x^4$ with ad-hoc $P(h,m)$

Search for TTLS in experiments and numerical simulations



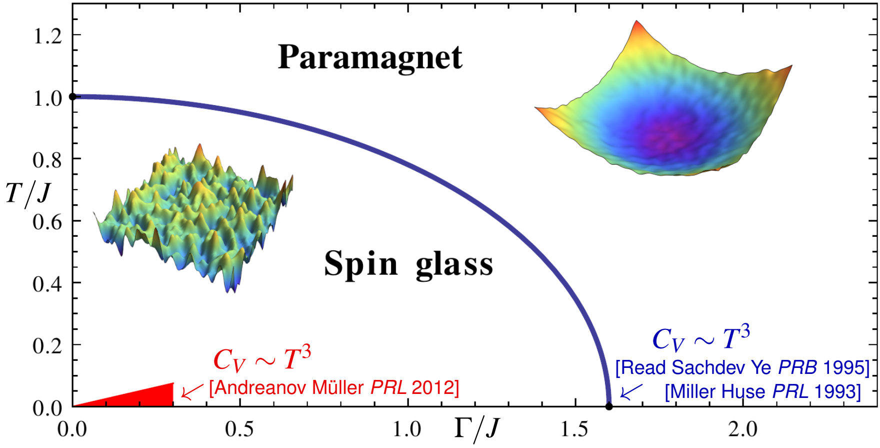


[Mocanu, Berthier, Ciarella, Khomenko, Reichman, Scalliet, Zamponi `arXiv:2209.09579`]

Mean-field models: a bit of history

Sherrington-Kirkpatrick in transverse field (SK):

$$\hat{H}_{\mathrm{SK}} = -\sum_{i<j} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z - \Gamma \sum_i \hat{\sigma}_i^x$$



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- Replica-symmetry breaking (RSB) terms must be included
  $\Rightarrow C_V \sim T$ inside the glass phase in SK and $SU(N \to \infty)$ Heisenberg
  [Georges Parcollet Sachdev *PRB* 2001] [Cugliandolo, Grempel, da Silva Santos, *PRB* 2001]

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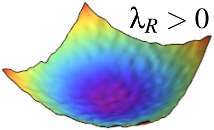
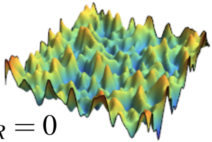


Systematic perturbative expansion:

$\hbar \to 0$ with $\beta\hbar$ fixed



Mechanism:

replicon $\lambda_R = 0 \Rightarrow C_V \sim T^3$ in many glass models
(including $SU(N \to \infty)$ Heisenberg, not SK!)

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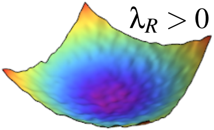

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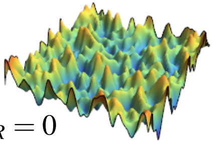

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  + diluted SK (Viana-Bray) hosts localized vibrations $\to$ TTLS?

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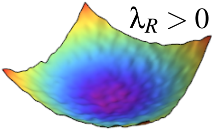

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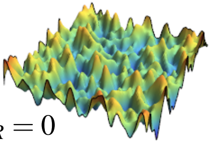

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Low-energy excitations in mean-field quantum spin glasses (such as SK) seem not entirely understood

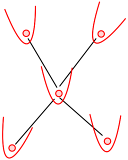
KHGPS model: solvable in the classical $T \to 0$ limit

Following in particular R. Kühn's works

$$H = \sum_{i<j}^{1,N} J_{ij} x_i x_j + \sum_{i=1}^{N} \frac{x_i^4}{4!} + \frac{\kappa_i}{2} x_i^2 - h x_i$$

Gaussian $\overline{J_{ij}^2} = J^2/N$, $p(\kappa)$ uniform in $[\kappa_m > 0, \kappa_M]$

[Bouchbinder Lerner Rainone Urbani Zamponi *PRB* 2021]



[Folena Urbani *JSTAT* 2021]
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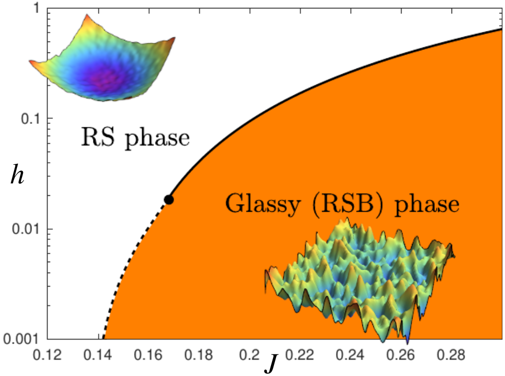

Classical $T = 0$ phase diagram

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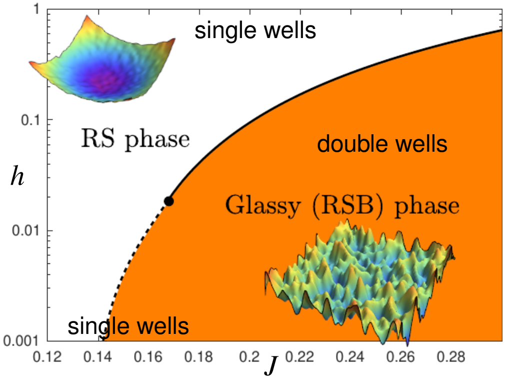

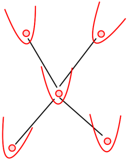

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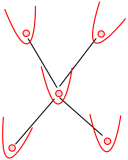

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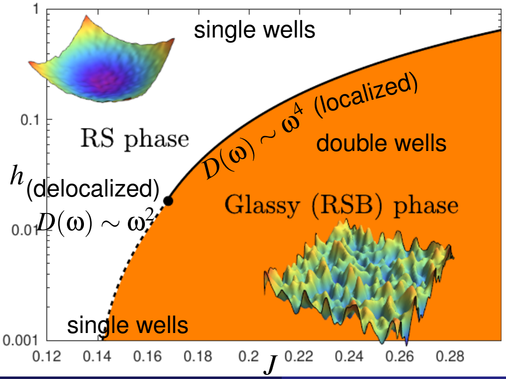
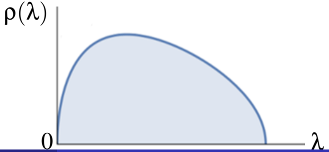


Hessian in an energy minimum

$$\partial^2_{ij} H = \overbrace{J_{ij}}^{\text{GOE}} + \left(\kappa_i + \frac{(x_i^*)^2}{2} \right) \delta_{ij}$$

eigenvalue density $\rho(\lambda)$

$\to$ vibrational DOS $D(\omega = \sqrt{\lambda})$



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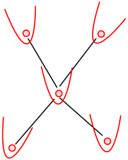

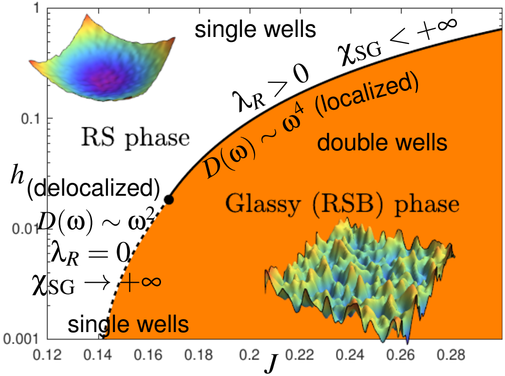

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Spin-glass susceptibility

$$\chi_{SG} = \frac{1}{N} \sum_{ij} \Big(\langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle \Big)^2$$

$$\chi_{SG} \sim \frac{1}{N} \mathrm{Tr} \left(\partial^2 H \right)^{-2} = \int \mathrm{d}\lambda \frac{\rho(\lambda)}{\lambda^2}$$

Quantized KHGPS

$$\hat{H}=\sum_{i=1}^{N}\frac{\hat{p}_i^2}{2M}+\sum_{i<j}^{1,N}J_{ij}\hat{x}_i\hat{x}_j+\sum_{i=1}^{N}\frac{\hat{x}_i^4}{4!}+\frac{\kappa_i}{2}\hat{x}_i^2-h\hat{x}_i\,,\quad [\hat{x}_i,\hat{p}_i]=i\hbar\delta_{ij}$$

Partition function: Matsubara periodic trajectories in imaginary time $t\in[0,\beta\hbar]$

Disorder average (replicas) + large N: order parameter $q_{ab}(t,s)=\frac{1}{N}\sum_i\left\langle x_i^a(t)x_i^b(s)\right\rangle$

$$\frac{U}{N}=\mathcal{U}[q_{ab}(t)]-\int \mathrm{d}p(\kappa)\mathrm{d}H\,P_\kappa(H)\frac{\partial}{\partial\beta}\ln\oint \mathrm{D}x\,e^{\mathcal{A}[x]}$$

Effective action

$$\mathcal{A}[x]=\frac{J^2}{2\hbar^2}\int_0^{\beta\hbar}\mathrm{d}t\mathrm{d}s\,x(t)G(t-s)x(s)-\frac{1}{\hbar}\int_0^{\beta\hbar}\mathrm{d}t\left[\frac{M}{2}\dot{x}^2+\frac{x^4}{4!}+\frac{\kappa}{2}x^2-Hx\right]$$

Large N saddle-point equations with *self-consistent* structure

$$G(t-s)=\int \mathrm{d}p(\kappa)\mathrm{d}H\,P_\kappa(H)\left(\left\langle x(t)x(s)\right\rangle-\left\langle x(t)\right\rangle\left\langle x(s)\right\rangle\right)$$

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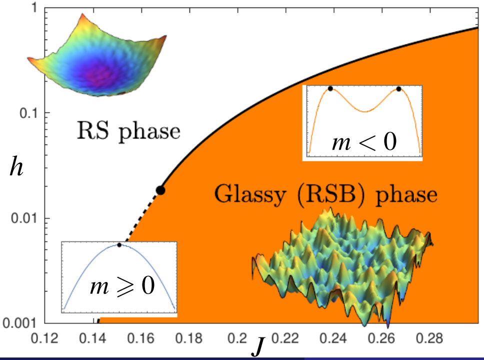
Strategy: SGLD expansion $\hbar \to 0$ at fixed $\beta\hbar$

$\hbar \to 0$ at fixed $\beta\hbar$ expansion

Saddle-point asymptotic expansion of averages

$$M\ddot{x}(t) = -J^2 \int_0^{\beta\hbar} \mathrm{d}s \, \frac{G(t-s)}{\hbar} x(s) + \frac{\partial}{\partial x(t)} \left[\frac{x(t)^4}{4!} + \frac{\kappa}{2} x(t)^2 - Hx(t) \right]$$

Static solutions : extrema of $\frac{x^4}{4!} + \frac{m}{2}x^2 - Hx$ with $m \equiv \kappa - J^2 \int_0^{\beta\hbar} G/\hbar$



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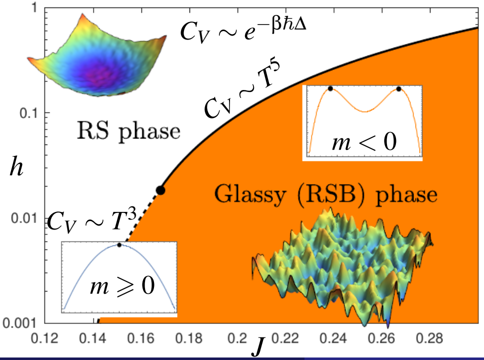

If unique static solution

$$\frac{U}{N} = e_{\mathrm{GS}}^{\mathrm{cl}} - \int_0^{\infty} D(\omega)\mathrm{d}\omega \, \hbar\omega \left(f_{\mathrm{B}}(\omega) + \frac{1}{2} \right) + O(\hbar^2)$$

$$D(\omega) = -\frac{2M\omega}{\pi} \operatorname{Im} \widetilde{G}(-i\omega + 0^+)$$

'disordered' Debye holds at lowest order due to gaplessness + RMT $\neq$ SGLD mechanism $\lambda_{\mathbf{R}} = 0$

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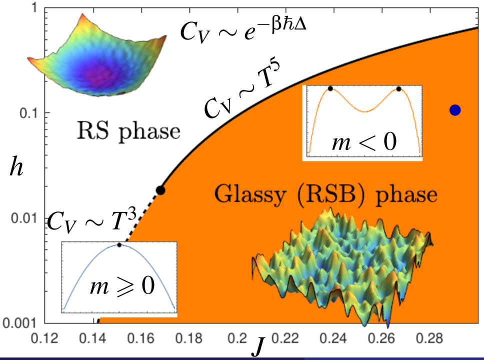

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2 static solutions: instantons

Variational free energy

$F\left[q_{a\neq b}, G(t)\right] \to F\left[q_{a\neq b}, \chi = \int_0^{\beta\hbar} G/\hbar\right]$

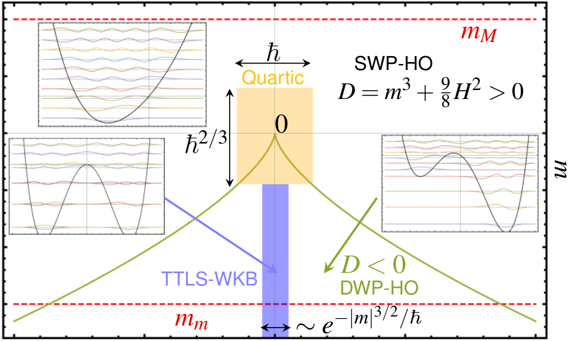
$\to$ solve self-consistent equations for $q_{a\neq b}, \chi, P_\kappa(H)\ldots$

$$\ln \oint \mathrm{D}x\, e^{\mathcal{A}[x]} \to \mathrm{Tr} e^{-\beta \hat{H}_{\mathrm{eff}}}$$

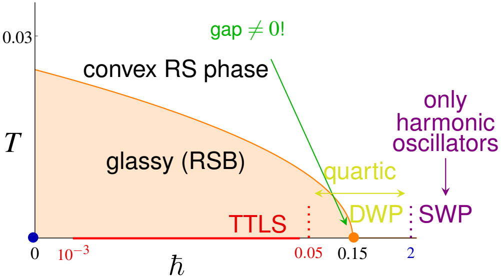
$$\hat{H}_{\mathrm{eff}} = \frac{\hat{p}^2}{2M} + \frac{\hat{x}^4}{4!} + \frac{m}{2}\hat{x}^2 - H\hat{x}$$

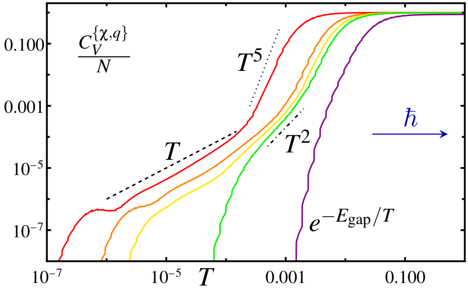
$$\frac{U^a}{N} = f\left(q_{a\neq b}, \chi\right) + \int \mathrm{d}p(m)\mathrm{d}H\, P_\kappa(H) \left\langle \hat{H}_{\mathrm{eff}} \right\rangle_H, \quad m \equiv \kappa - J^2\chi$$

Solvable for
$\hbar$ finite and T $\to 0$



Numerical/analytical results in the variational treatment





variational approximation
$\Rightarrow$ energy gap cannot vanish
$\Rightarrow$ factor $e^{-E_{\mathrm{gap}}/T}$ in C_V at low enough T

Beyond: lessons from the spin-boson model

Need for full imaginary-time dependence when instantons are present

$$\mathcal{A}[x] = \frac{J^2}{2\hbar^2}\int_0^{\beta\hbar} \mathrm{d}t\mathrm{d}s\, x(t)G(t-s)x(s) - \frac{1}{\hbar}\int_0^{\beta\hbar}\mathrm{d}t\left[\frac{M}{2}\dot{x}^2 + \frac{x^4}{4!} + \frac{\kappa}{2}x^2 - Hx\right]$$

$$G(t-s) = \int \mathrm{d}p(\kappa)\mathrm{d}H\, P_\kappa(H)\left(\langle x(t)x(s)\rangle - \langle x(t)\rangle\langle x(s)\rangle\right)$$

Assume we have solved for $\widetilde{G}(\omega) \sim \omega^s \to$ *approximate* mapping to Caldeira-Leggett:

$$\widetilde{H} = \frac{\hat{p}^2}{2M} + \frac{\hat{x}^4}{4!} + \frac{\kappa}{2}\hat{x}^2 - H\hat{x} + \sum_\alpha \frac{\hat{p}_\alpha^2}{2m_\alpha} + \frac{m_\alpha\omega_\alpha^2}{2}\hat{x}_\alpha^2 - c_\alpha\hat{x}_\alpha\hat{x}$$

Symmetric double wells at low T: mapped to spin-boson model

$$\widetilde{H} \sim \frac{\Delta_0}{2}\hat{\sigma}_x - \frac{1}{2}\hat{\sigma}_z\sum_\alpha \hbar\lambda_\alpha(\hat{b}_\alpha + \hat{b}_\alpha^\dagger) + \sum_\alpha \hbar\omega_\alpha\hat{b}_\alpha^\dagger\hat{b}_\alpha$$

with bath spectral function $\sim \widetilde{G}(\omega)$

For $s \leqslant 1$ renormalization by the bath modes
$\Rightarrow$ vanishing gap $\Delta_0 = 0$ (localization) and $C_V \sim T^s$

[Bray Moore *PRL* 1982, Charkravarty *PRL* 1982, Gorlich Weiss *PRB* 1988]

Conclusions

- Need for better understanding of low-energy excitations in quantum mean-field glasses
- KHGPS good mean-field model for finite-dimensional aspects of glasses
- KHGPS quantum thermodynamics has consistent features of delocalized soft harmonic excitations (Debye-like), localized classical non-linear excitations and tunneling two-level systems
- Clearer physical picture of semiclassical expansion $\hbar \to 0$ with $\beta\hbar$ fixed:

  1. no instantons $\Rightarrow$ critical scaling ruled by RMT (a disordered version of Debye theory)
  2. instantons $\Rightarrow$ physics closer to the TTLS picture

- Full imaginary-time solution needed in the instantonic regime to find true criticality and possibly interesting physics phenomena like localization

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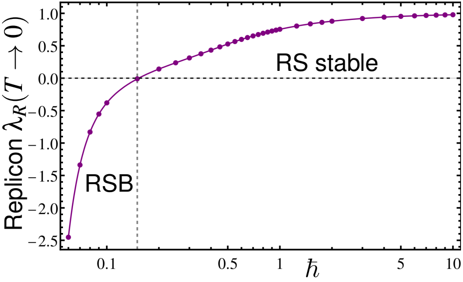
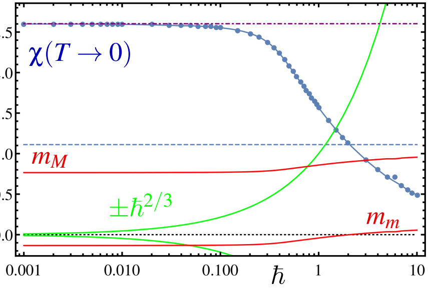
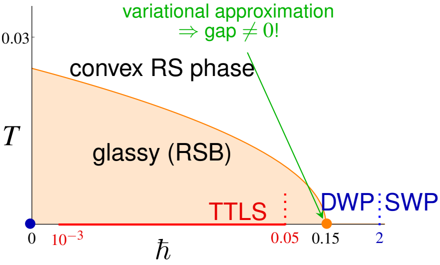
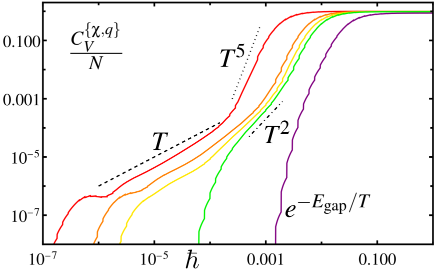
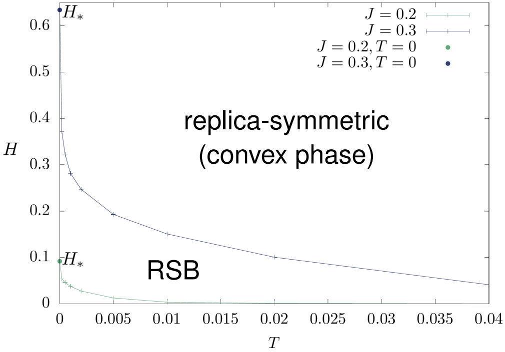


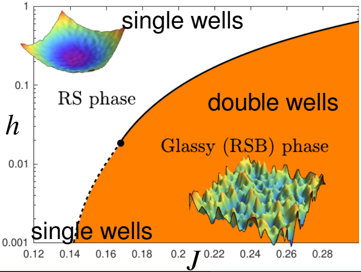






KHGPS model: transition in a field at $T = 0$



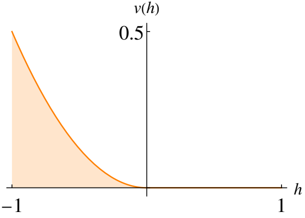


$$H = \sum_{i<j}^{1,N} J_{ij} x_i x_j + \sum_{i=1}^{N} \frac{x_i^4}{4!} + \frac{\kappa_i}{2} x_i^2 - h x_i$$

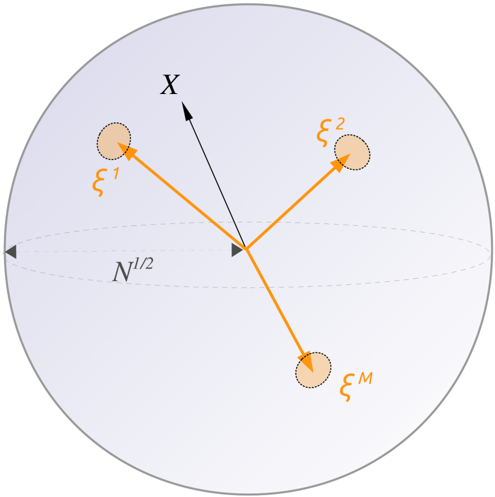
Classical spherical perceptron

- $\mathbf{X} = (X_1, \ldots, X_N) \quad N \to \infty$
  on a sphere $\mathbf{X}^2 = N$
- Random obstacles $\boldsymbol{\xi}^\mu$, $\mu \in [\![1, M]\!]$
  density $\alpha = M/N$
- $H = \sum_{\mu=1}^{M} v(\underbrace{r_\mu(\mathbf{X}) - \sigma}_{\text{"interparticle gap"}})$

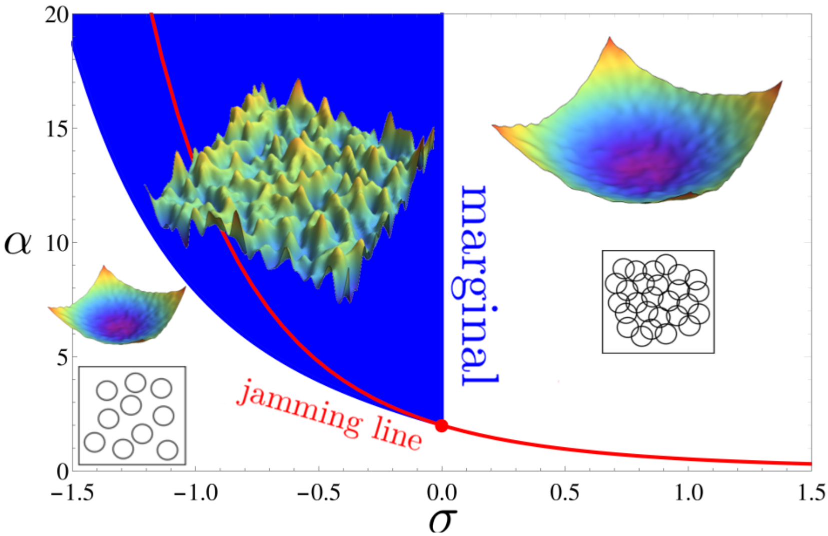
$$r_\mu(\mathbf{X}) = \frac{\boldsymbol{\xi}^\mu \cdot \mathbf{X}}{\sqrt{N}}$$



$\sigma < 0$: **non-convex phase**



Classical phase diagram at $T = 0$

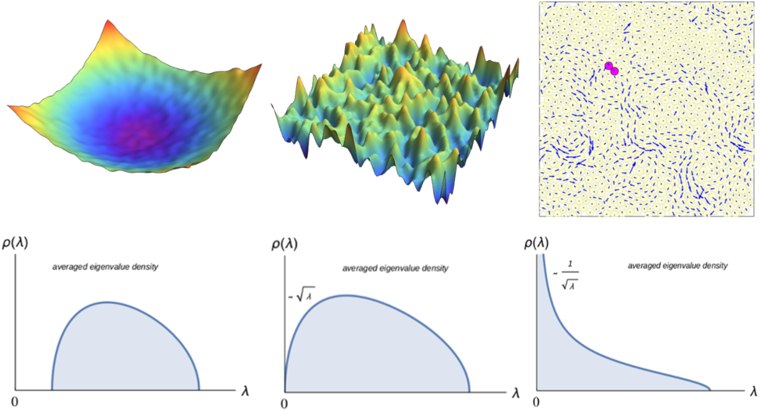


[Franz, Parisi *JPhysA* 2016], [Franz, Parisi, Sevelev, Urbani, Zamponi *SciPost* 2017]

Debye approximation and vibrational spectrum

$$C_V = \frac{\partial}{\partial T} \int_0^\infty \mathrm{d}\omega D(\omega) \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}$$

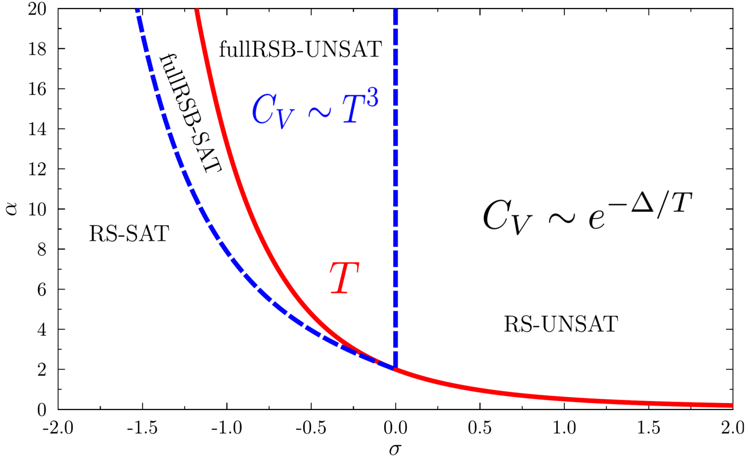
Density of vibrational modes $D(\omega)$: $m\omega^2 = \lambda$ eigenvalue of $\partial^2 H / \partial X_i \partial X_j$



[Franz, Parisi, Urbani, Zamponi *PNAS* 2015]

Debye approximation for $T \to 0$ in the overjammed phase

$$C_V = \frac{\partial}{\partial T} \int_0^\infty \mathrm{d}\omega D(\omega) \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}$$



Pitfalls of the Debye approximation

1. At jamming, extensive number of soft modes !

2. The jamming transition should become a crossover for $\hbar > 0$

Specific heat from the free energy

Quantum version of the perceptron:

$$[X_i, P_j] = i\hbar\delta_{ij}$$

$$\hat{H} = \frac{\hat{\mathbf{P}}^2}{2m} + \sum_{\mu=1}^{M} v(r_\mu(\hat{\mathbf{X}}) - \sigma)$$

Schehr-Le Doussal-Giamarchi (2004) expansion:

$\hbar \to 0$ **with fixed Matsubara period** $\beta\hbar \Rightarrow T \sim \hbar \to 0$

provides mechanism for scaling in T valid at all orders

Imaginary-time action: $-\frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau \left[\frac{m}{2}\dot{\mathbf{X}}^2 + \sum_\mu v(h_\mu(\mathbf{X}))\right]$

Thermodynamic energy:

$$\frac{U_{\text{tot}}}{N} = \underbrace{u_{(0)}(\beta\hbar)}_{\text{classical ground state}} + \hbar u_{(1)}(\beta\hbar) + O(\hbar^2)$$

Low-temperature specific heat in the overjammed phase

Single-basin phase: gapped $C_V \sim e^{-\Delta/T}$

(Landscape) marginally stable phase: $\Delta = 0$ $\quad (\Rightarrow C_V =$ power law$)$

Finite $\hbar$: in the whole marginal phase

$$C_V \propto \frac{T}{\hbar} \mathcal{F}\left(T/T_{\text{cut}}\right) \propto \frac{T^3}{T_{\text{cut}}^2 + T^2}$$

- $\exists$ cutoff temperature T_{cut} $\qquad$ ($\delta =$ distance to jamming)

$$T_{\text{cut}} \propto \underbrace{\sqrt{\frac{\varepsilon}{m} \frac{\hbar}{k_B \mathcal{D}}}}_{\approx 1\text{ K}} \sqrt{\delta} + \underbrace{O(\hbar^2)}_{\approx 0.01\text{ K}}$$

$$T \ll T_{\text{cut}} \;\Rightarrow\; C_V \propto T^3$$
$$T \gg T_{\text{cut}} \;\Rightarrow\; C_V \propto T$$

Low-temperature specific heat in the overjammed phase

Finite $\hbar$: in the whole marginal phase

$$C_V \propto \frac{T}{\hbar}\mathcal{F}\left(T/T_{\rm cut}\right) \propto \frac{T^3}{T_{\rm cut}^2 + T^2}$$

- ∃ cutoff temperature $T_{\rm cut}$

$$T_{\rm cut} \propto \underbrace{\sqrt{\frac{\varepsilon}{m}\frac{\hbar}{k_{\rm B}\mathcal{D}}}}_{\approx 1\ \rm K}\sqrt{\delta} + \underbrace{O(\hbar^2)}_{\approx 0.01\ \rm K}$$

($\delta =$ distance to jamming)

$$T \ll T_{\rm cut} \ \Rightarrow\ C_V \propto T^3$$
$$T \gg T_{\rm cut} \ \Rightarrow\ C_V \propto T$$

Summary:

- Marginal landscape brings soft glassy modes, entails a power-law C_V and excess C_V w.r.t. the crystal
- Depending on the value of $T_{\rm cut}$, due to avoided jamming criticality, one may observe the linear scaling.
  More likely if the system is close to the classical jamming line
- Debye approximation does not hold close to jamming
- Jamming becomes a crossover for $\hbar \to 0$