Nonlinear Gibbs measure and equilibrium Bose gases

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Goal

Nonlinear Gibbs measure

$$d\mu(u) = \text{``}z^{-1} \exp\left[-\beta\left(\int_\Omega |\nabla u|^2 + \kappa|u|^2 + |u|^2(w * |u|^2)\right)\right] du\text{''}$$

invariant under NLS flow

$$i\dot{u} = (-\Delta + \kappa)u + (w * |u|^2)u$$

used in

- Euclidean Quantum Field Theory (Glimm-Jaffe, Simon '70s, ...)
- NLS equation with rough initial data (Lebowitz-Rose-Speer '88, Bourgain '90s, Burq-Thomann-Tzvetkov '00s, ...)
- Stochastic PDE (da Prato-Debbussche '03, Hairer '14, ...)

Goal: μ arised from many-body quantum mechanics, in a mean-field limit

Difficulty: μ is singular, energy functional is $+\infty$ almost everywhere

Gibbs measure

Free (Gaussian) measuse

$h = -\Delta + \kappa > 0$ on bounded domain $\Omega \subset \mathbb{R}^d$, $hu_j = \lambda_j u_j$. Then

$$d\mu_0(u) = \text{``}z_0^{-1} e^{-\langle u, hu\rangle} du\text{''} := \bigotimes_{j\geq 1} \left(\frac{\lambda_j}{\pi} e^{-\lambda_j |\alpha_j|^2} d\alpha_j \right), \quad \alpha_j = \langle u_j, u\rangle \in \mathbb{C}$$

is well defined on Sobolev space H^s if and only if $s < 1 - d/2$

Interacting measure

$$d\mu(u) = \text{``}z^{-1} e^{-\langle u, hu\rangle - \mathcal{D}(u)} du\text{''} := z_r^{-1} e^{-\mathcal{D}(u)} d\mu_0(u)$$

is well-defined when

- $d = 1$, $0 \leq w \in a\delta_0 + L^\infty$ and
$$\mathcal{D}(u) = \frac{1}{2} \iint w(x-y)|u(x)|^2 |u(y)|^2 dxdy$$
- $d = 2, 3$, $0 \leq \widehat{w} \in L^1$ and
$$\mathcal{D}(u) = \frac{1}{2} \iint w(x-y) \Big(|u(x)|^2 - \langle |u(x)|^2 \rangle_{\mu_0} \Big) \Big(|u(y)|^2 - \langle |u(y)|^2 \rangle_{\mu_0} \Big)$$

Many-body quantum model

Bosonic Gibbs state

$$\Gamma_{\lambda,T} = Z_{\lambda,T}^{-1} e^{-H_\lambda/T}$$

with grand-canonical Hamiltonian

$$H_\lambda = \bigoplus_{n=0}^{\infty} \left(\sum_{j=1}^{n} (-\Delta_{x_j} + \kappa) + \lambda \sum_{1 \le i < j \le n} w(x_i - x_j) \right) \quad \text{on} \quad \bigoplus_{n=0}^{\infty} L^2_{sym}(\Omega^n)$$

$$= \int a_x^* (-\Delta + \kappa) a_x dx + \frac{\lambda}{2} \iint w(x-y) a_x^* a_y^* a_x a_y dxdy$$

Mean-field limit $\lambda = T^{-1} \to 0$ formally leads to **semiclassical approximation**

$$Z_{T^{-1},T} = \operatorname{Tr} \exp \left[-\frac{1}{T} \int a_x^* (-\Delta + \kappa) a_x dx - \frac{1}{2T^2} \iint w(x-y) a_x^* a_y^* a_x a_y dxdy \right]$$

$$\sim \quad (T/\pi)^{\dim L^2(\Omega)} \int_{L^2(\Omega)} e^{-\int \overline{u(x)} (-\Delta + \kappa) u(x) dx - \frac{1}{2} \iint w(x-y) |u(x)|^2 |u(y)|^2 dxdy} du$$

1D result

$$\Gamma_{\lambda,T} = Z_{\lambda,T}^{-1} \exp\left[-\frac{1}{T}\int a_x^*(-\Delta+\kappa)a_x\,dx - \frac{\lambda}{2T}\iint w(x-y)a_x^*a_y^*a_xa_y\,dxdy\right]$$

Theorem (Lewin-N-Rougerie '15)

Assume $d=1$, $0 \le w \in a\delta_0 + L^\infty$ and $\lambda = T^{-1} \to 0$. Then

$$\frac{Z_{\lambda,T}}{Z_{0,T}} \to z_r = \int_{L^2(\Omega)} e^{-\mathcal{D}(u)}d\mu_0(u)$$

and

$$\frac{k!}{T^k}\Gamma_{\lambda,T}^{(k)} \to \int_{L^2(\Omega)} |u^{\otimes k}\rangle\langle u^{\otimes k}|d\mu(u), \quad \forall k \ge 1$$

strongly in trace class

Remarks

- Reduced density matrices $\Gamma_{\lambda,T}^{(k)}(x_1,...,x_k;y_1,...,y_k) = \mathrm{Tr}[a_{x_1}^*...a_{x_k}^*a_{y_1}...a_{y_k}\Gamma_{\lambda,T}]$
- Fragmentation of Bose-Einstein condensates
- μ determined completely by all moments

Renormalized Hamiltonian $d \geq 2$

$$\mathcal{D}(u) = \frac{1}{2} \iint w(x-y)\Big(|u(x)|^2 - \langle |u(x)|^2 \rangle_{\mu_0}\Big)\Big(|u(y)|^2 - \langle |u(y)|^2 \rangle_{\mu_0}\Big)$$

$$= \frac{1}{2} \int \widehat{w}(k) \left| \int_\Omega |u(x)|^2 e^{ik\cdot x} dx - \left\langle \int_\Omega |u(x)|^2 e^{ik\cdot x} dx \right\rangle_{\mu_0} \right|^2 dk$$

$$\rightsquigarrow H_\lambda = \int a_x^*(-\Delta + \kappa) a_x dx + \frac{\lambda}{2} \int \widehat{w}(k) \left| \mathrm{d}\Gamma(e^{ik\cdot x}) - \langle \mathrm{d}\Gamma(e^{ik\cdot x}) \rangle_{\Gamma_{0,T}} \right|^2 dk$$

$$= \int a_x^*(-\Delta + V_T(x)) a_x dx + \frac{\lambda}{2} \iint w(x-y) a_x^* a_y^* a_x a_y dx dy + \frac{\lambda}{2} \langle \rho_{0,T}, w * \rho_{0,T} \rangle$$

with $\quad V_T(x) = \kappa + \lambda w(0)/2 - \lambda w * \rho_{0,T}(x), \quad \rho_{0,T}(x) = \left[\frac{1}{e^{\frac{-\Delta+\kappa}{T}} - 1} \right](x;x)$

In **homogeneous case** ($-\Delta_{\mathrm{periodic}}$ on unit torus)

$$\rho_{0,T}(x) = \sum_{k \in (2\pi\mathbb{Z})^d} \frac{1}{e^{\frac{|k|^2+\kappa}{T}} - 1} \sim \begin{cases} T & \text{in } d = 1 \\ T \log T & \text{in } d = 2 \\ T^{3/2} & \text{in } d = 3 \end{cases}$$

and V_T is simply a (modified) chemical potential

2D result

$$\Gamma_{\lambda,T} = Z_{\lambda,T}^{-1} \exp\left[-\frac{\int a_x^*(-\Delta + V_T(x))a_x dx + \frac{\lambda}{2}\iint w(x-y)a_x^* a_y^* a_x a_y dxdy + E_T}{T}\right]$$

Theorem (Lewin-N-Rougerie '18)

Assume $d = 2$, $0 \leq \widehat{w}(k)(1 + |k|) \in L^1$ and $\lambda = T^{-1} \to 0$. Then

$$\frac{Z_{\lambda,T}}{Z_{0,T}} \to z_r = \int e^{-\mathcal{D}(u)} d\mu_0(u)$$

and

$$\frac{k!}{T^k}\Gamma_{\lambda,T}^{(k)} \to \int |u^{\otimes k}\rangle\langle u^{\otimes k}| d\mu(u), \quad \forall k \geq 1$$

strongly in Schatten space $\mathfrak{S}^p$ for all $p > 1$. Moreover,

$$\frac{\Gamma_{\lambda,T}^{(1)} - \Gamma_{0,T}^{(1)}}{T} \to \int |u^{\otimes k}\rangle\langle u^{\otimes k}|(d\mu(u) - d\mu_0(u)) \quad \text{in trace class}$$

Similar result expected in $d = 3$ (work in progress)

Remarks

- Fröhlich-Knowles-Schlein-Sohinger 2017: μ arised in $d \leq 3$ for

$$e^{-\varepsilon H_0/T} e^{-(H_\lambda - 2\varepsilon H_0)/T} e^{-\varepsilon H_0/T}$$

- Rescaling $T \mapsto 1$ and $\Omega \mapsto [0, L]^d$ with $L \to \infty$: free density

$$\frac{1}{L^d} \sum_{k \in 2\pi\mathbb{Z}^d} \frac{1}{e^{\frac{k^2+\kappa}{L^2}} - 1} \to \rho_c = \begin{cases} +\infty & \text{in } d = 1, 2 \\ \int_{\mathbb{R}^3} \frac{1}{e^{|2\pi k|^2} - 1} dk & \text{in } d = 3 \end{cases}$$

  Thus the Gibbs measure tells us the behavior **just below the critical density**, or equivalently **just above the critical temperature** for BEC

- Deuchert-Seiringer-Yngvason 2018: BEC transition in thermodynamic and Gross-Pitaevskii limit

Ideas of proofs

Variational approach:

$$\Gamma_{\lambda,T} \text{ minimizes} \qquad -\log \frac{Z_{\lambda,T}}{Z_{0,T}} = \inf_{\Gamma \geq 0, \operatorname{Tr}\Gamma = 1} \Big[\underbrace{\mathcal{H}(\Gamma, \Gamma_{0,T})}_{\operatorname{Tr}(\Gamma(\log\Gamma - \log\Gamma_{0,T}))} + \frac{\lambda}{T} \operatorname{Tr}(\mathbb{W}\Gamma) \Big]$$

$$\mu \text{ minimizes} \qquad -\log z_r = \inf_{\nu \text{ prob. measure}} \Big[\underbrace{\mathcal{H}_{\rm cl}(\nu, \mu_0)}_{\int \frac{d\nu}{d\mu_0} \log \frac{d\nu}{d\mu_0} d\mu_0} + \int \mathcal{D}(u) d\nu(u) \Big]$$

Quantum to classical by quantum de Finetti theorem

$$\frac{k!}{T^k} \Gamma^{(k)}_{\lambda,T} \rightharpoonup \int |u^{\otimes k}\rangle\langle u^{\otimes k}| d\nu(u), \quad \forall k \geq 1$$

In $d = 1$ the result essentially follows from

$$\liminf \mathcal{H}(\Gamma_{\lambda,T}, \Gamma_{0,T}) \geq \mathcal{H}_{\rm cl}(\nu, \mu_0) \qquad \text{(Berezin-Lieb)}$$

$$\liminf \frac{\lambda}{T} \operatorname{Tr}(\mathbb{W}\Gamma_{\lambda,T}) = \liminf \frac{1}{T^2} \operatorname{Tr}(w\Gamma^{(2)}_{\lambda,T}) \geq \int \mathcal{D}(u) d\nu(u) \qquad \text{(Fatou)}$$

Ideas of proofs

For $d \geq 2$, renormalized interaction has no sign $\rightsquigarrow$ Fatou's lemma fails to apply!

Localization method

$$\Gamma_{\lambda,T} \approx (\Gamma_{\lambda,T})_P \otimes (\Gamma_{0,T})_Q, \quad P = \mathbb{1}(-\Delta + \kappa \leq \Lambda), Q = 1 - P$$

Use quantitative de Finetti for P modes, and error estimate for Q modes

Lemma (Variance estimate: $d = 2, \Lambda \geq T^\delta$)

$$\frac{1}{T^2}\left\langle \left(\mathrm{d}\Gamma(Q) - \langle \mathrm{d}\Gamma(Q)\rangle_{\Gamma_{\lambda,T}} \right)^2 \right\rangle_{\Gamma_{\lambda,T}} \to 0$$

Proof. Reduce two-body to one-body problem

$$\left\langle \left(\mathrm{d}\Gamma(Q) - \langle \mathrm{d}\Gamma(Q)\rangle_{\lambda,T} \right)^2 \right\rangle_{\Gamma_{\lambda,T}} \approx T\partial_{\varepsilon=0} \frac{\mathrm{Tr}\left[\mathrm{d}\Gamma(Q) e^{-\frac{\mathbb{H}_\lambda - \varepsilon \mathrm{d}\Gamma(Q)}{T}}\right]}{\mathrm{Tr}\left[e^{-\frac{\mathbb{H}_\lambda - \varepsilon \mathrm{d}\Gamma(Q)}{T}}\right]},$$

then control $g'(0)$ by $g(\varepsilon) - g(0)$ and g'', thanks to Taylor's expansion

$$g(\varepsilon) = g(0) + g'(0)\varepsilon + \frac{\varepsilon^2}{2} g''(\theta_\varepsilon)$$