Fluctuation-induced forces in confined He and Bose gases

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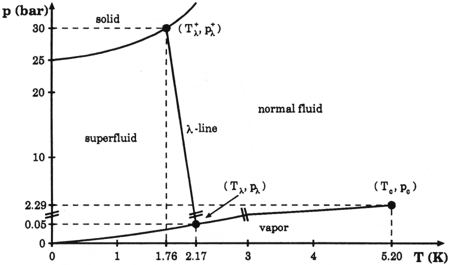
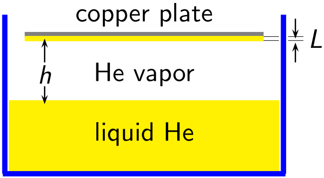
PRE **91**, 062114 (2015); *JPA Math & Theor.* **48**, 375201 (2015); and to be published

Thinning of ^{4}He wetting films





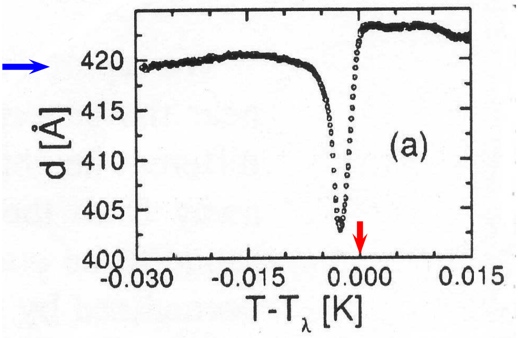
$$\boxed{\underbrace{mgh}_{\text{gravitation}} = \underbrace{\frac{\gamma_{\mathrm{vdW}}}{L^3}}_{\text{van der Waals}} \underbrace{\frac{1}{1+L/L_{1/2}}}_{\text{retardation}} + \underbrace{v\, k_B T\, \frac{\vartheta(x)}{L^3}}_{\text{“Casimir”}}}$$

$$f_L \equiv \lim_{A\to\infty} \beta F(T,L)/A = L\, f_{\mathrm{b}}(T) + f_{\mathrm{s}}(T) + f_{\mathrm{res}}(T,L)$$

$$f_{\mathrm{res}}(T,L) = L^{-(d-1)}\,\Theta(x)\,, \quad x = t(L/\xi_+)^{1/\nu}$$

$$\underbrace{\beta\mathcal{F}_C(T,L)}_{\text{fluctuation-induced force}} = -\partial_L f_{\mathrm{res}}(T,L) = L^{-d}\,\vartheta(x)$$

Thinning of ^{4}He films near T_λ



Experiment:
Garcia & Chan, *PRL* **83**, 1187 (1999)

- Theory: ?
  - Krech & Dietrich 1991/92: $T \geq T_\lambda$, ϵ expansion
  - Li & Kardar 1991: $T \ll T_\lambda$ (noninteracting Goldstone modes)
  - Zandi, Rudnick & Kardar 2004: interface fluctuations
  - Monte Carlo simulations: A. Hucht (PRL 2007); Vasilyev, Gambassi, Maciołek & Dietrich (EPL 2007); M. Hasenbusch JSTAT 2009, PRB 2010

Thinning of ^{4}He wetting layers

(iii) ⇳

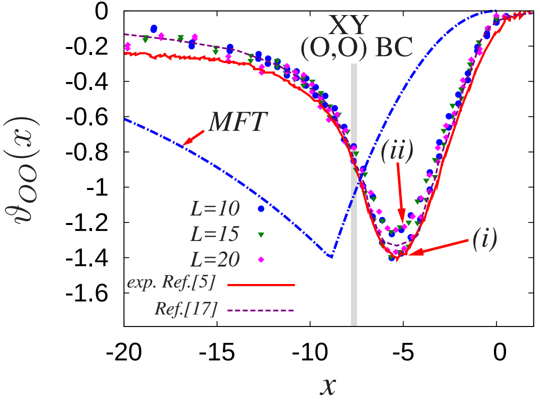
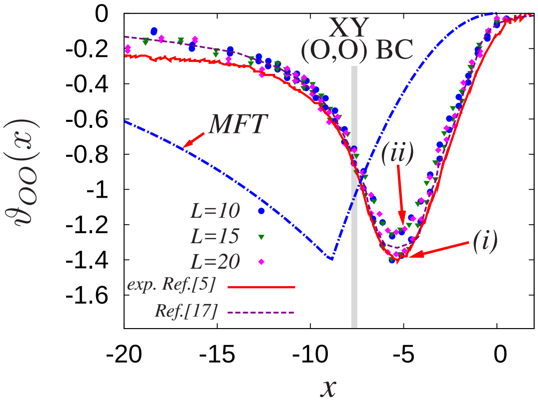


Fig 4 of (ii) Vasilyev *et al*: *PRE* **79**, 041142, (2009)
(i) A. Hucht: *PRL* **99**, 185301 (2007).
MFT: Zandi *et al*: *PRE* **76**, 030601 (2007) & (ii);
Experiments: Garcia & M.H.W. Chan: *PRL*, **83** (1999);
Ganshin, Scheidemantel, Garcia & Chan. *PRL*, **97**, 075301 (2006).

Thinning of ^{4}He wetting layers



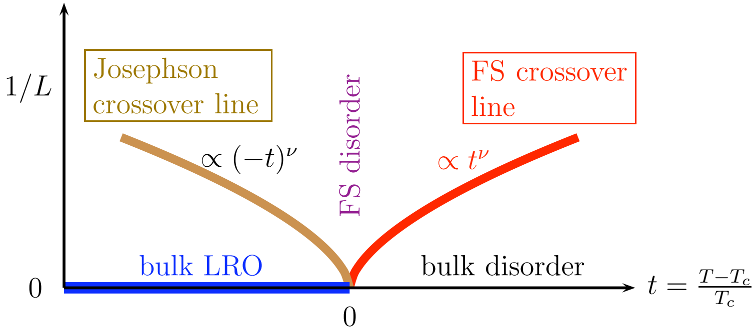
(RG-improved) MFT is qualitatively wrong

- predicts sharp finite-L transition
- predicts incorrect low-T behavior, $\lim_{T\to 0}\mathcal{F}_{\mathrm{C}} \to 0$
  no "nonperturbative mass generation" for finite L
- predicts jump discontinuity of $\vartheta'(x)$ at $x_{\min}$

Finite-L $O(n)$ phase diagram for $d = 3$

$$\mathcal{H} = \int_{\mathbb{R}^{d-1}\times[0,L]} \mathrm{d}^d r \left[\frac{1}{2}(\nabla\phi)^2 + \frac{\mathring{\tau}}{2}\phi^2 + \frac{g}{4!n}\phi^4\right] + \text{boundary terms}$$

$n < \infty$



$$\xi_L(t \to -\infty) \sim \mathrm{e}^{\mathrm{const}\, L|t|^{\nu}}$$

Finite-L $O(n)$ phase diagram for $d = 3$

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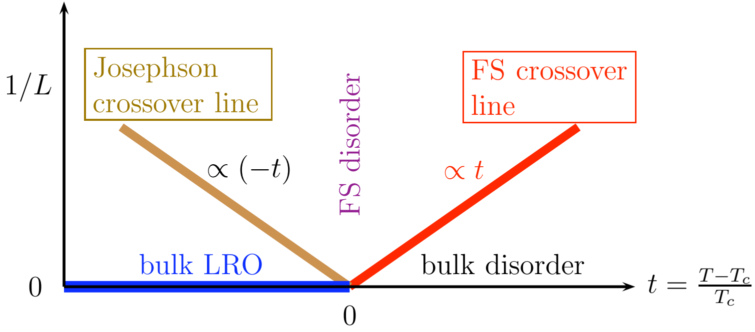
$$n = \infty; \quad \nu = \tfrac{1}{d-2} \overset{d=3}{=} 1$$



$$\xi_L(t \to -\infty) \sim \mathrm{e}^{\mathrm{const}\, L|t|^{\nu}}$$

Exact $n = \infty$ solution

- $f_L \equiv \lim_{n\to\infty} \lim_{A\to\infty} \frac{-\ln \mathcal{Z}}{An}$

$$f_L = \frac{1}{2} \int_{\boldsymbol{p}}^{(d-1)} \sum_\nu \ln(p^2 + \epsilon_\nu) - \frac{3}{2g} \int_0^L \mathrm{d}z\, [\mathring{\tau} - v(z)]^2$$

$$[-\partial_z^2 + v(z)]\varphi_\nu(z) = \epsilon_\nu\, \varphi_\nu(z)$$

$$\frac{\delta f_L}{\delta v(z)} \stackrel{!}{=} 0 \Rightarrow \boxed{\mathring{\tau} - v(z) =}$$

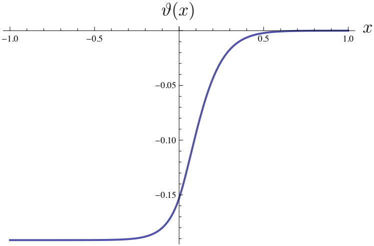
$$\boxed{= -\frac{g}{6} \int_{\boldsymbol{p}}^{(d-1)} \sum_\nu \frac{|\varphi_\nu(z)|^2}{\boldsymbol{p}^2 + \epsilon_\nu}}$$

self-consistency condition!

- exact closed-form solution known for periodic boundary conditions at $d = 3$ (Danchev 1996)

Exact $n \to \infty$ solution?

- Yes for periodic boundary conditions: $v(z) \equiv v_b$
  exact closed-form solution known for $d = 3$ (Danchev *PRE* **53**, 2104 1996)



$\Longrightarrow$ free boundary conditions important!

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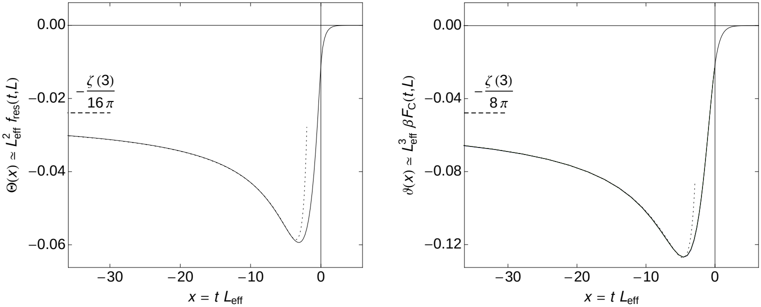
  $\Longrightarrow$ free boundary conditions important!

- free boundary conditions: by numerical means

  $\Longrightarrow$ "numerically exact results" for Θ and ϑ for $T - T_c \gtreqless 0$ and $L < \infty$



HWD, Grüneberg, Hasenbusch, Hucht, Rutkevich, Schmidt: *EPL* **100**, 10004 (2012); *PRE* **89**, 62123 (2014); **91**, 026101 (2015)
cf also: Dantchev *et al* *PRE* **89** 04216 (2014)

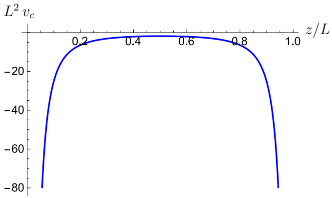
Exact analytical solutions possible?

- Difficulty: $v(z)$ = singular at surface planes!

$$v(z;L,t) \underset{z\to 0}{=} \underbrace{-\frac{1}{4z^2}}_{\text{Bray \& Moore '77}} + \underbrace{\frac{4t}{\pi^2 z}}_{\text{HWD \& SBR '14}} + \underbrace{\frac{56\,\zeta(3)}{\pi^4}\,t^2}_{\substack{\text{SBR \& HWD '15}\\ \text{new trace formula}}} + \dots$$

  Proper self-adjoint extension? Several lengths: z, $1/|t|$, L!

- Critical potential:



- Distant-wall correction:

$$v(z;L,0) \underset{z\ll L}{=} \frac{(d-3)^2-1}{4z^2}\Big[1 + \overbrace{B_d\,(z/L)^d}^{\text{distant-wall correction}}\Big]$$

$\underbrace{\text{BOE \& SDE}}_{\text{HWD \& SBR '14}}$ + results from Cardy and McAvity & Osborne

$$\Longrightarrow\quad \boxed{B_3 = -\frac{1024}{\pi}\,\Delta_C}\,,\quad \Delta_C = \Theta(0) = -0.010773406850247\,82(1)$$

Inverse scattering approach ($L = \infty$)

$$\varphi(\mathsf{z}, \mathsf{k}) \underset{\mathsf{z}\to\infty}{\simeq} \frac{A(\mathsf{k})}{\mathsf{k}} \sin[\mathsf{kz} + \eta(\mathsf{k})]$$

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$$\varphi(\mathsf{z},\mathsf{k}) \underset{\mathsf{z}\to\infty}{\simeq} \frac{A(\mathsf{k})}{\mathsf{k}} \sin[\mathsf{kz} + \eta(\mathsf{k})]$$

- Self-consistency equation: $\boxed{\delta f[v_*, \delta v] = \int_0^\infty \mathrm{d}z\, \frac{\delta f[v]}{\delta v_*(z)}\, \delta v(z) \stackrel{!}{=} 0}$.
- Express δv in terms of $\delta\eta_\pm(\mathsf{k})$, $\sigma_\pm(\mathsf{k}) = \ln \mathsf{A}_\pm(\mathsf{k})$, where $\mathsf{k} = k/|t|$ $(t \gtrless 0)$.
- $\delta\sigma_\pm(\mathsf{k}) \xleftrightarrow{\text{Kramers-Kronig}} \delta\eta_\pm(\mathsf{k})$
- $\Longrightarrow$ Integral equations for $\sigma_\pm(\mathsf{k})$

Inverse scattering approach ($L=\infty$)

$$\varphi(\mathsf{z},\mathsf{k}) \underset{\mathsf{z}\to\infty}{\simeq} \frac{A(\mathsf{k})}{\mathsf{k}} \sin[\mathsf{kz}+\eta(\mathsf{k})]$$

- Self-consistency equation: $\delta f[v_*,\delta v] = \int_0^\infty \mathrm{d}z \, \frac{\delta f[v]}{\delta v_*(z)} \, \delta v(z) \overset{!}{=} 0$.
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- $\delta\sigma_\pm(\mathsf{k}) \xleftrightarrow{\text{Kramers-Kronig}} \delta\eta_\pm(\mathsf{k})$
- $\Longrightarrow$ Integral equations for $\sigma_\pm(\mathsf{k})$

$$\begin{aligned}
A_+(\mathsf{k}) &= \sqrt{\frac{\mathsf{k}}{\arctan \mathsf{k}}}, \quad \eta_+(\mathsf{k}) = \int_0^\infty \mathrm{du}\, \frac{2\arctan(\mathsf{k}\tanh \mathsf{u})}{4\mathsf{u}^2+\pi^2}, \\
A_-(\mathsf{k}) &= \frac{|\mathsf{k}|}{\sqrt{1+\pi|\mathsf{k}|/2}}, \\
\eta_-(\mathsf{k}) &= \mathrm{sgn}(\mathsf{k}) \left\{ \frac{\pi}{2} + \frac{1}{2\pi} \left[\mathrm{Li}_2\left(-\frac{\pi|\mathsf{k}|}{2}\right) - \mathrm{Li}_2\left(\frac{\pi|\mathsf{k}|}{2}\right) - \ln\left(\frac{\pi|\mathsf{k}|}{2}\right) \ln \frac{2-\pi|\mathsf{k}|}{2+\pi|\mathsf{k}|} \right] \right\}
\end{aligned}$$

- $\Longrightarrow$ **Jost functions exactly known!**
- $v(z)$ could be reconstructed from scattering data (Povzner, Levitan, Marchenko integral equation)

Exact phase shifts for all temperature values $t \gtreqless 0$

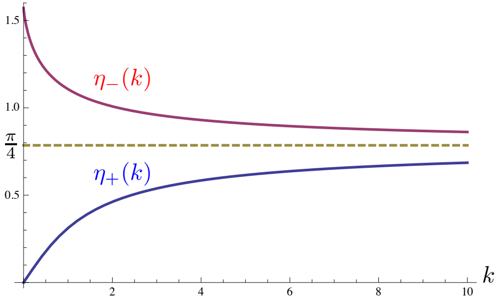


Figure: Phase shifts η_-(k) for $t < 0$ (red) and η_+(k) for $t \geq 0$ (blue), and $t = 0$ (yellow)

S. B. Rutkevich and H. W. Diehl, *PRE* **91**, 062114 (2015)

Other exact analytical results

- Exact two-point correlation functions $G^{(2)}(\boldsymbol{y}, z, z'; \infty, m)$, $G^{(0,2)}(\boldsymbol{y}; \infty, m)$, and bulk correlation function $G_{\mathrm{b}}^{(2)}(\boldsymbol{x}; m)$, $z_\pm \equiv z \pm z'$ and $\boldsymbol{x} = (\boldsymbol{y}, z)$.

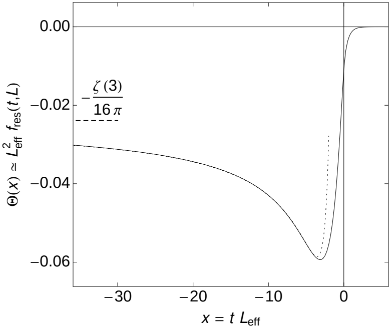
	$G^{(2)}(\boldsymbol{y}, z, z')$	$G^{(0,2)}(\boldsymbol{y})$	$G_{\mathrm{b}}^{(2)}(\boldsymbol{x})$
$t > 0$		$\frac{1}{2\pi y^2}\,\mathrm{e}^{-ty}$	$\frac{1}{4\pi x}\,\mathrm{e}^{-tx}$
$t = 0$	$\frac{\sqrt{zz'}}{2\pi\sqrt{(y^2+z_+^2)(y^2+z_-^2)}}$	$\frac{1}{2\pi y^2}$	$\frac{1}{4\pi x}$
$t < 0$		$\frac{1}{2\pi y^2} + \frac{\lvert t\rvert}{2\pi y} + \frac{t^2}{4\pi}$	$\frac{1}{4\pi x} + \frac{\lvert t\rvert}{4\pi}$

- Thermal singularity of surface free energy: $\Longrightarrow\ \vartheta''(0) = -\pi^{-3}$.
- Universal amplitude difference of surface free energy
- Properly defined excess order parameter

Exact $n = \infty$ Casimir force scaling function for free boundary conditions and $d = 3$

- introduce $x = \left[L/\xi_{\rm b}^+\right]^{1/\nu}\tau = \frac{24\pi\tau}{g}L = tL$ with $\nu = \frac{1}{d-2} \underset{d=3}{=} 1$
- selfconsistent equations (A): $t = \langle z|\ln \boldsymbol{H}|z\rangle$

$$f_{\rm ex}(L,t) = \frac{1}{8\pi}\mathrm{Tr}[\boldsymbol{H}\,(1+t-\ln \boldsymbol{H})] - L\frac{t}{4\pi} - L\,\underbrace{\frac{\theta(t)}{4\pi}[\sinh(t)-t]}_{=f_b(t)}$$



- $L = 2^5, \ldots, 2^8$
- data collapse in scaling plot
- low-T behavior:
  $d_1 = 2\left[\gamma_{\rm E} + \ln\frac{4}{\pi}\right] - 1 - 2\frac{\zeta'(3)}{\zeta(3)}$
  $= 0.967205644660601\ldots$

$$\Theta(x) \underset{x\to-\infty}{\simeq} -\frac{\zeta(3)}{16\pi}\left[1 + \frac{d_1 + 2\ln|x|}{|x|} + o(|x|^{-1})\right]$$

Exact $L < \infty$ results

- Inverse-Scattering Approach + Matched semi-classical expansions $\Longrightarrow$

1. Exact $x \to -\infty$ asymptotic behavior of $\Theta(x)$ & $\vartheta(x)$

$$\boxed{\Theta(x) \underset{x\to-\infty}{\simeq} -\frac{\zeta(3)}{16\pi}\left[1 + \frac{d_1 + 2\ln|x|}{|x|} + o(|x|^{-1})\right]}$$

$$d_1 = 2\left[\gamma_E + \ln\frac{4}{\pi}\right] - 1 - 2\frac{\zeta'(3)}{\zeta(3)} = 0.967205644660601\ldots$$

2. Exact $x \to -\infty$ asymptotic behavior of scaled eigenstates and eigenfunctions

$$\begin{aligned} E_1(x) &\underset{x\to-\infty}{=} (e/\pi)\,|x|\,\mathrm{e}^{-|x|+o(1/|x|^0)} \\ E_{\nu>1}(x) &\underset{x\to-\infty}{=} \pi^2(\nu-1)^2\left[1 + 2|x|^{-1}\ln|x|\right] + O(1/|x|). \end{aligned}$$

- Further exact results:

3. Thermal singularity of surface free energy: $\boxed{\Longrightarrow\ \vartheta''(0) = -\pi^{-3}}$.
4. Universal amplitude difference of surface free energy
5. Properly defined excess order parameter

Confined ideal and interacting bosons

$$\hat{H} = \frac{\hbar^2}{2m}\int_{\mathfrak{V}}[\nabla\hat{\psi}^\dagger(\boldsymbol{x})]\nabla\hat{\psi}(\boldsymbol{x}) + \frac{1}{2}\int_{\mathfrak{V}\times\mathfrak{V}}\hat{\psi}^\dagger(\boldsymbol{x})\hat{\psi}^\dagger(\boldsymbol{x}')u(\boldsymbol{x}-\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x})$$

- usual choice: $u(\boldsymbol{x}) = \mathring{u}\,\delta(\boldsymbol{x})$
- commutation relations:

$$[\hat{\psi}(\boldsymbol{x}),\hat{\psi}^\dagger(\boldsymbol{x})] = \delta(\boldsymbol{x}-\boldsymbol{x}'), \qquad [\hat{\psi}(\boldsymbol{x}),\hat{\psi}(\boldsymbol{x})] = [\hat{\psi}^\dagger(\boldsymbol{x}),\hat{\psi}^\dagger(\boldsymbol{x})] = 0.$$

- boundary conditions $(\mathrm{BC} = \mathrm{per},\mathrm{ap},\mathrm{DD},\mathrm{NN},\mathrm{DN},\mathrm{R})$:

$$\hat{\psi}^{\mathrm{BC}}(\boldsymbol{r},z) = \sum_k \mathfrak{h}_k^{\mathrm{BC}}(z)\int\frac{\mathrm{d}^{d-1}\boldsymbol{p}}{(2\pi)^{(d-1)/2}}\,\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\,b_{\boldsymbol{p},k}$$

$$\mathfrak{h}_k^{\mathrm{DN}}(0) = 0, \quad \partial_z\mathfrak{h}_k^{\mathrm{DN}}(L) = 0, \quad (\partial_z - c_1)\mathfrak{h}_k^{\mathrm{R}}(0) = 0$$

Boson models

1. ideal: $u(\boldsymbol{x}) = 0$
2. imperfect: PE $\approx a\frac{N(N-1)}{2V} = a\frac{N^2}{2V}[1 + O(N^{-1})]$
3. n internal degrees of freedom:

$$\hat{H} = \frac{\hbar^2}{2m}\int_{\mathfrak{V}}[\nabla\hat{\psi}^\dagger_\alpha(\boldsymbol{x})]\nabla\hat{\psi}_\alpha(\boldsymbol{x}) + \frac{\mathring{u}}{2n}\int_{\mathfrak{V}}\hat{\psi}^\dagger_\alpha(\boldsymbol{x})\hat{\psi}^\dagger_\beta(\boldsymbol{x})\hat{\psi}_\beta(\boldsymbol{x})\hat{\psi}_\alpha(\boldsymbol{x})$$

- commutation relations:

$$[\hat{\psi}_\alpha(\boldsymbol{x}), \hat{\psi}^\dagger_\beta(\boldsymbol{x})] = \delta_{\alpha\beta}\,\delta(\boldsymbol{x}-\boldsymbol{x}'), \quad [\hat{\psi}_\alpha(\boldsymbol{x}), \hat{\psi}_\beta(\boldsymbol{x})] = [\hat{\psi}^\dagger_\alpha(\boldsymbol{x}), \hat{\psi}^\dagger_\beta(\boldsymbol{x})] = 0.$$

Ideal Bose-gas case

- grand partition sum: $\Xi_d(T,\mu,L,L_\parallel) = \mathrm{Tr}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}$
- grand reduced potential per cross-sectional area $L_\parallel^{d-1}$:

$$\begin{aligned}\varphi_d^{\mathrm{BC}}(T,\mu,L) &= -\lim_{L_\parallel\to\infty} \frac{1}{L_\parallel^{d-1}} \ln \Xi_d^{\mathrm{BC}}(T,\mu,L,L_\parallel) \\ &= L\varphi_{d,\mathrm{b}}(T,\mu) + \varphi_{d,\mathrm{s}}^{\mathrm{BC}}(T,\mu) + \varphi_{d,\mathrm{res}}^{\mathrm{BC}}(T,\mu,L)\end{aligned}$$

- length scales:
  1. thermal de-Broglie wavelength: $\lambda_{\mathrm{th}} = \hbar\sqrt{2\pi\beta/m}$
  2. correlation length: $\xi = \dfrac{\hbar}{\sqrt{2m(-\mu)}}$

$$\varphi_{d,\mathrm{res}}^{\mathrm{BC}}(T,\mu,L) = L^{-(d-1)}\Upsilon_d^{\mathrm{BC}}(L/\lambda_{\mathrm{th}}, L/\xi)$$

$$\begin{aligned}\varphi_{d,\mathrm{b}}(T,\mu) &= -\lambda_{\mathrm{th}}^{-d}\mathrm{Li}_{\frac{d+2}{2}}(\mathrm{e}^{-\hbar^2/2m\xi^2}) \\ &= -\varphi_{d,\mathrm{s}}^{\mathrm{NN}}(T,\mu) = \tfrac{1}{2}\lambda_{\mathrm{th}}^{-(d-1)}\mathrm{Li}_{\frac{d+1}{2}}\left(\mathrm{e}^{-\lambda_{\mathrm{th}}^2/4\pi\xi^2}\right)\end{aligned}$$

Ideal Bose-gas case II

- residual grand potential:

$$\boxed{\varphi^{\mathrm{BC}}_{d,\mathrm{res}}(T,\mu,L) = L^{-(d-1)}\Upsilon^{\mathrm{BC}}_d(L/\lambda_{\mathrm{th}}, L/\xi)}$$

- $d > 2 \implies T_c > 0$: quantum effects should not matter in critical regime!

$$\Upsilon^{\mathrm{BC}}_d(x_\lambda, x_\xi) \underset{x_\lambda \to \infty}{\approx} \Upsilon^{\mathrm{BC}}_d(\infty, x_\xi) = \underbrace{\Theta^{\mathrm{BC}}_d(x_\xi)}_{O(2)\text{ free field theory}}$$

$d = 3$: Martin & Zagrebnov 06, Gambassi & Dietrich 06;
$d > 2$, HWD & SBR 16

$$\Theta^{\mathrm{DD}}_3(x_\xi) = \Theta^{\mathrm{NN}}_3(x_\xi) = -\frac{1}{8\pi}\left[\mathrm{Li}_3(\mathrm{e}^{-2x_\xi}) + 2x_\xi\,\mathrm{Li}_2(\mathrm{e}^{-2x_\xi})\right]$$

- critical exponents? $\nu_{\mathrm{bg}} = \frac{1}{d-2} \neq \nu_{\mathrm{G}} = \frac{1}{2}$, $\eta_{\mathrm{bg}} = 0$

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- critical exponents? $\nu_{\mathrm{bg}} = \frac{1}{d-2} \neq \nu_{\mathrm{G}} = \frac{1}{2}$, $\eta_{\mathrm{bg}} = 0$
- density ρ fixed, not $\mu \implies$ Fisher-renormalized exponents

$$\nu_{\mathrm{bg}} = \frac{\nu_{\mathrm{G}}}{1-\alpha_{\mathrm{G}}} = \frac{1/2}{1-(2-d/2)} = \frac{1}{d-2}$$

Imperfect Bose gas

- $\hat{H} = \int\limits_{\mathbb{R}^{d-1}\times[0,L]} \left[\frac{\hbar^2}{2m}\nabla\hat{\psi}^\dagger \cdot \nabla\hat{\psi}\right] + a\frac{\hat{N}^2}{2V}$
- exact solution under periodic BC (Jacubczyk & Napiorkowski 13) $\leftrightarrow$ saddle-point evaluation of contour integral
- main findings:
  1. critical exponents = spherical-model exponents
  2. Casimir amplitude $\Delta_C^{\text{impbg}} = 2\Delta_C^{\text{sph}}$

     $\Delta_C^{\text{sph}} = \lim_{n\to\infty} \frac{1}{n}\Delta_C^{O(n)}$
  3. scaling function

$$\Theta_d^{\text{impbg}}(x_\xi) \stackrel{?}{=} 2\Theta^{\text{sph}}(x_\xi)$$

Universality class?

Answers (HWD & SBR 16):

- Imperfect BG corresponds to $n \to \infty$ limit of n-state interacting BG

$$\hat{H} = \frac{\hbar^2}{2m}\int_{\mathfrak{V}}[\nabla\hat{\psi}^\dagger_\alpha(\boldsymbol{x})]\nabla\hat{\psi}_\alpha(\boldsymbol{x}) + \frac{\mathring{u}}{2n}\int_{\mathfrak{V}}\hat{\psi}^\dagger_\alpha(\boldsymbol{x})\hat{\psi}^\dagger_\beta(\boldsymbol{x})\hat{\psi}_\beta(\boldsymbol{x})\hat{\psi}_\alpha(\boldsymbol{x})$$

- Consequences:
  1. UC(impbg) $=$ UC[$O(2\infty)$-model]
     2 because BG order parameter $\in \mathbb{C}$
  2. holds for (leading) critical behavior of $\varphi^{\mathrm{per}}_{d,\mathrm{b}}$ and $\varphi^{\mathrm{per}}_{d,\mathrm{res}}$!
  3. $\Longrightarrow$ natural non-translation invariant generalizations of imperfect BG models for BC $=$ DD, NN, DN, R.
     Scaling functions Θ^{BC}_d of $O(2\infty)$ models
  4. quantum fluctuations: exponentially small corrections

Conclusions

1. Classical systems:
   - large-n limit of classical $O(n)$ theory can simultaneously handle:
     (i) bulk, surface, and finite-size critical behavior,
     (ii) dimensional crossover,
     (iii) low-T Goldstone fluctuations
   - All qualitative features of $\Theta(x)$ for ^{4}He (XY) case recovered:
   - exact analytical results for fluctuation-induced forces by a combination of methods
   - Full finite-size scaling functions by numerical means
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Thank you for your attention!