Variational Perturbation Theory

Converting Divergent Weak-Coupling Expansions into Exponentially Fast Convergent Strong-Coupling Expansions

Hagen Kleinert, FU BERLI & ICRANet Pesc

Roots

Rayleigh-Ritz-Prinzip

John William Strutt, 3. Baron Rayleigh (1842 –1919)
Nobel Prize 1904)

Walter Ritz
(1878 –1909)

Hartree-Fock Theory

D. R. Hartree
(1897 –1958)

W.A. Fock
(1898 –1974)

Higher Effective Action

Cyrano De Dominicis 1962

But no good in strong-coupling limit!

Principle of Minimal Sensitivity

P.M. Stevenson 1981

(Bridge to Seznec + Zinn-Justin 1979 previous lecture)

Effective Classical Partition Functions

PHYSICAL REVIEW A VOLUME 34, NUMBER 6 DECEMBER 1986

Effective classical partition functions

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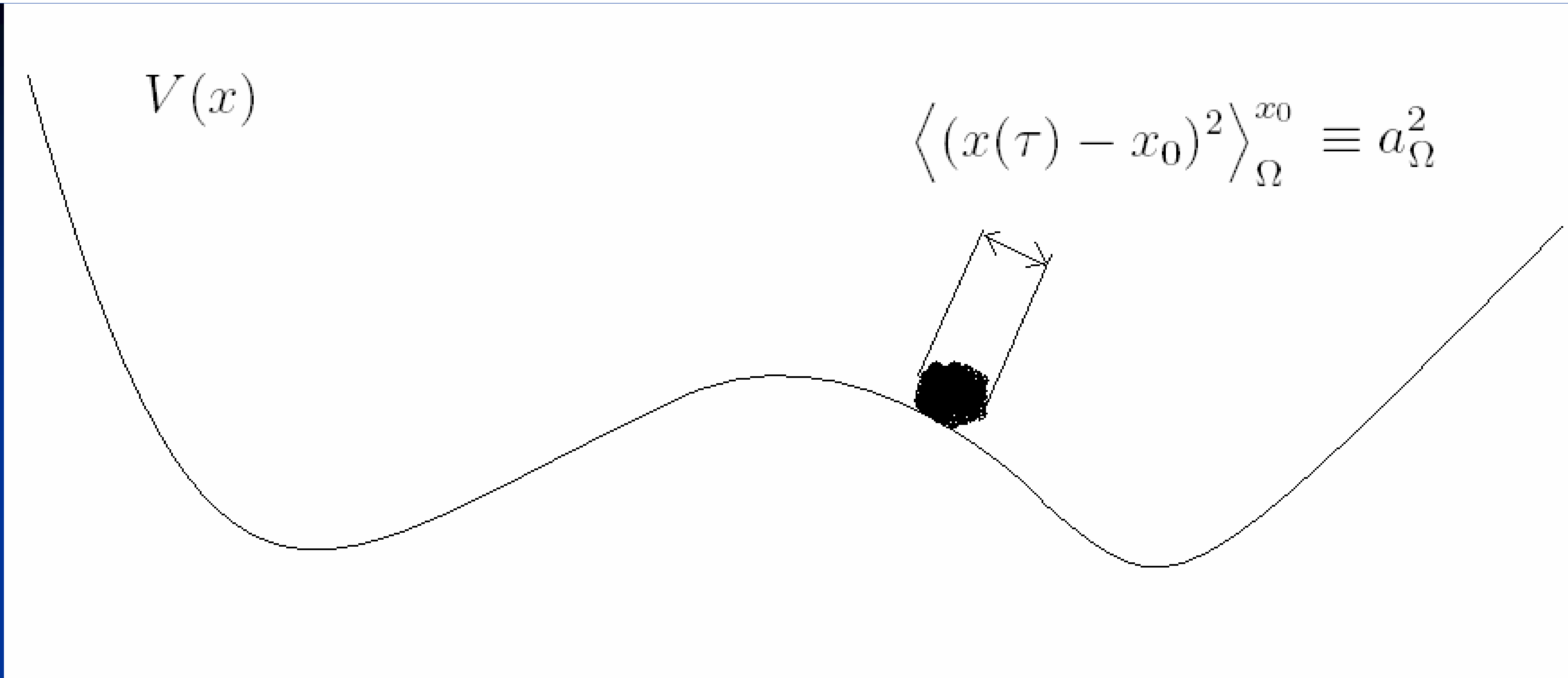
$$\mathcal{A}_{\rm e} = \int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{x}^2(\tau) + V(x(\tau))\right]$$

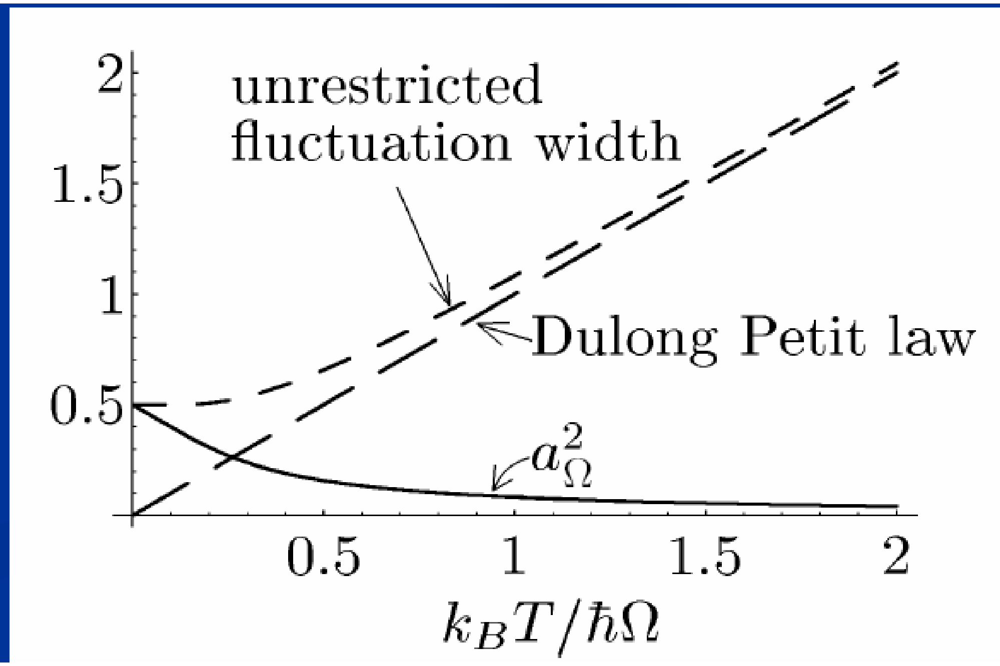
$$Z = \oint \mathcal{D}x\, e^{-\mathcal{A}_{\rm e}/\hbar} = \int_{-\infty}^{\infty} \frac{dx_0}{l_{\rm e}(\hbar\beta)} \oint \mathcal{D}'x\, e^{-\mathcal{A}_{\rm e}/\hbar} = \int_{-\infty}^{\infty} \frac{dx_0}{l_{\rm e}(\hbar\beta)} e^{-V^{\rm eff\ cl}(x_0)/k_BT}$$

$l_{\rm e}(\hbar\beta) \rightarrow \sqrt{2\pi\hbar^2\beta/M}$

$$B(x_0) \equiv e^{-V^{\rm eff\ cl}(x_0)/k_BT} = \oint \mathcal{D}'x\, e^{-\mathcal{A}_{\rm e}/\hbar} = \prod_{m=1}^{\infty} \left[\int \frac{dx_m^{\rm re} dx_m^{\rm im}}{\pi k_B T/M\omega_m^2}\right] \times$$
$$\times \exp\left[-\frac{M}{k_BT}\sum_{m=1}^{\infty}\omega_m^2|x_m|^2 - \frac{1}{\hbar}\int_0^{\hbar/k_BT} d\tau V\left(x_0 + \sum_{m=1}^{\infty}(x_m e^{-i\omega_m\tau} + \text{c.c.})\right)\right]$$



$$a_\Omega^2 \equiv \frac{1}{2\Omega}\coth\frac{\Omega\hbar\beta}{2} - \frac{1}{\hbar\beta\Omega^2}$$



$$\mathcal{A}_\Omega^{x_0} = \int_0^{\hbar/k_BT} d\tau M \left[\frac{\dot{x}^2}{2} + \Omega^2(x_0)\frac{(x-x_0)^2}{2}\right]$$

$$\begin{aligned} e^{-V^{\text{eff cl}}(x_0)/k_BT} &= Z^{x_0} = \int \mathcal{D}x\,\tilde{\delta}(\bar{x}-x_0)e^{-\mathcal{A}/\hbar} \\ &\equiv \int \mathcal{D}x\,\tilde{\delta}(\bar{x}-x_0)e^{-\mathcal{A}_\Omega^{x_0}/\hbar}e^{-(\mathcal{A}-\mathcal{A}_\Omega^{x_0})/\hbar} \\ &= Z_\Omega^{x_0}\left\langle e^{-(\mathcal{A}-\mathcal{A}_\Omega^{x_0})/\hbar}\right\rangle_\Omega^{x_0}. \end{aligned}$$

$$B_\Omega(x_0) \equiv e^{-V^{\text{eff cl}}(x_0)/k_BT} = \frac{\hbar\Omega(x_0)/2k_BT}{\sinh[\hbar\Omega(x_0)/2k_BT]} \equiv Z_\Omega^{x_0}$$

$$\left\langle e^{-(\mathcal{A}-\mathcal{A}_\Omega^{x_0})/\hbar}\right\rangle_\Omega^{x_0} \geq e^{-\left\langle \mathcal{A}/\hbar-\mathcal{A}_\Omega^{x_0}/\hbar\right\rangle_\Omega^{x_0}}$$

Jensen-Peierls

$$V^{\text{eff cl}}(x_0) \leq F_\Omega^{x_0}(x_0) + k_BT\left\langle \mathcal{A}/\hbar - \mathcal{A}_\Omega^{x_0}/\hbar\right\rangle_\Omega^{x_0}$$

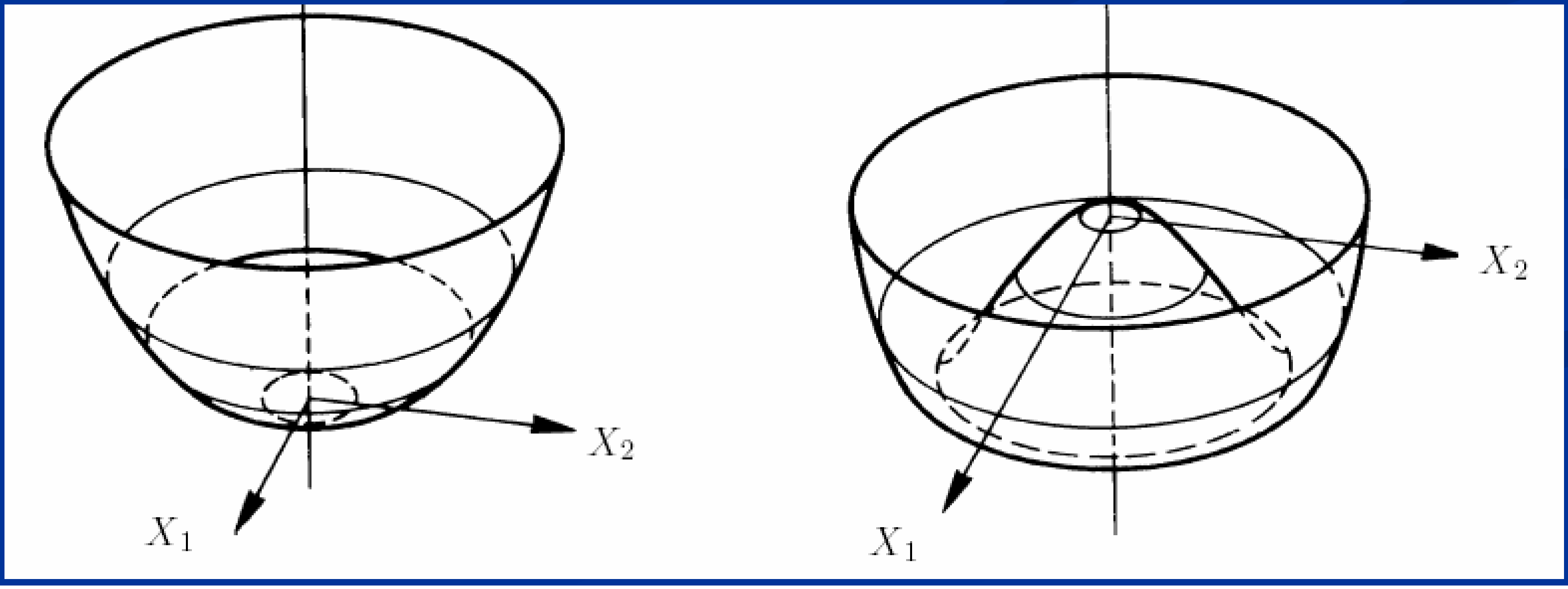
Solves Convexity Problem of Effective Action

$$Z[j] = e^{iW[j]/\hbar}$$

$$X(t) \equiv \langle x(t) \rangle = \delta W[j]/\delta j(t)$$

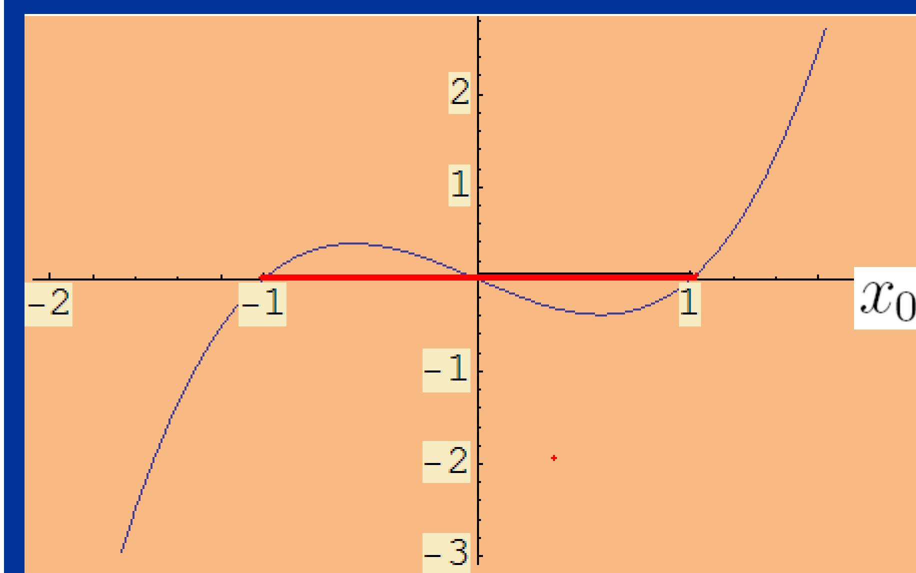
Legendre Transform

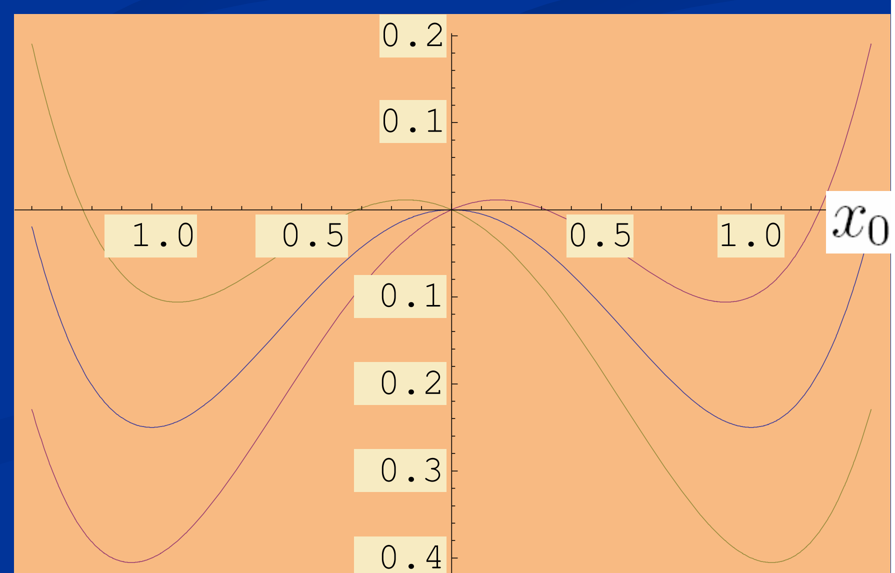
$$\Gamma[X] \equiv W[j] - \int dt\, j(t) X(t)$$



$$Z(j) = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta}} e^{-\beta[V^{\mathrm{eff\,cl}}(x_0) - jx_0]}$$

$$X = Z(j)^{-1} \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\beta}}\, x_0 \, \exp\left\{-\beta[V^{\mathrm{eff\,cl}}(x_0) - jx_0]\right\}$$





Can go to Higher-Order

Effective Classical Partition Functions

Exercise first at at T=0

Higher-Order

Variational Perturbation Theory (1990)

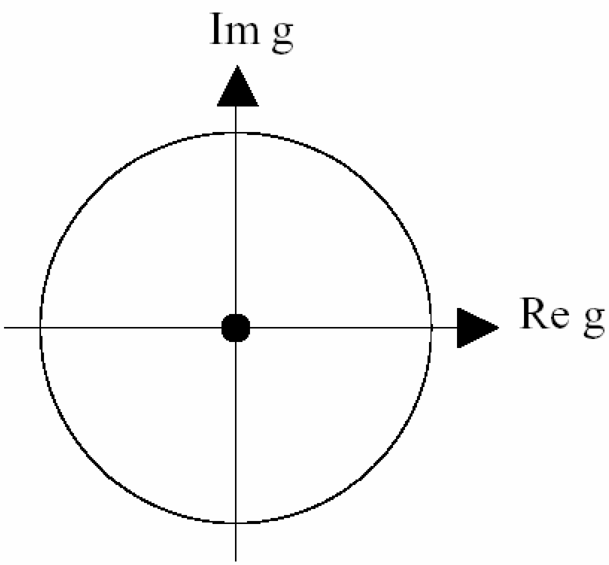
T=0

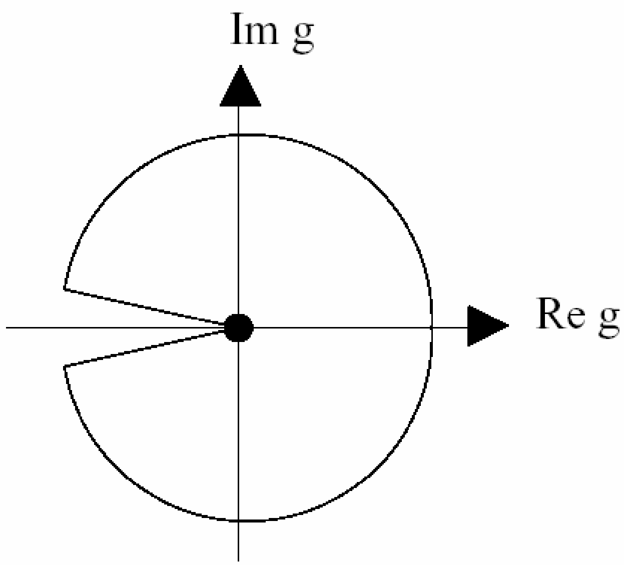
- Perturbation theory in QFT:

$$\Rightarrow \text{ weak-coupling series} \quad f_N(g) = \sum_{n=0}^{N} a_n \left(\frac{g}{m^{4-D}}\right)^n$$

$$\text{divergent since} \quad a_n \sim (-1)^n n!$$

- Analytic properties:





Dispersion relation:

$$f(g) = \frac{1}{\pi}\int_0^{\infty} dg' \frac{\mathrm{Im} f(-g')}{g'+g}$$

Hence

$$f_n = \frac{(-1)^n}{\pi}\int_0^{\infty} \frac{dg'}{g'^n} \mathrm{Im} f(-g')$$

Typical Problem

$$\mathrm{Im} f(-g') \propto e^{-a/g'}$$

Weak-coupling series: $f_N(g) = \sum_{n=0}^{N} a_n \, g^n$

variational perturbation theory yields strong-coupling limit

Strong-coupling series:

$$f_M(g) = g^{\frac{p}{q}} \sum_{m=0}^{M} b_m \, g^{-\frac{2}{q}m}$$

Anharmonic Oscillator

- Potential:

$$V(x) = \frac{1}{2}\omega^2 x^2 + g\,x^4$$

- Weak-coupling series of ground state energy:

$$E_0 = \frac{\omega}{2} + g\,\frac{3}{4\omega^2} - g^2\,\frac{21}{8\omega^5} + g^3\,\frac{333}{16\omega^8} + \dots$$

to any order via Bender-Wu recursion relations

- Insertion of an auxiliary harmonic oscillator:

$$V(x) = \frac{1}{2}\Omega^2 x^2 + g\,x^4 + \frac{1}{2}\left(\omega^2 - \Omega^2\right) x^2$$

Ω: variational parameter

- Square-root trick:

$$V(x) \;=\; \frac{1}{2}\omega^2 x^2 + g\,x^4, \quad \omega \equiv \sqrt{\Omega^2 + \omega^2 - \Omega^2}$$

$$\omega \;\Rightarrow\; \Omega\sqrt{1+gr}, \qquad r \equiv \frac{\omega^2 - \Omega^2}{g\Omega^2}$$

- Explicit first order:

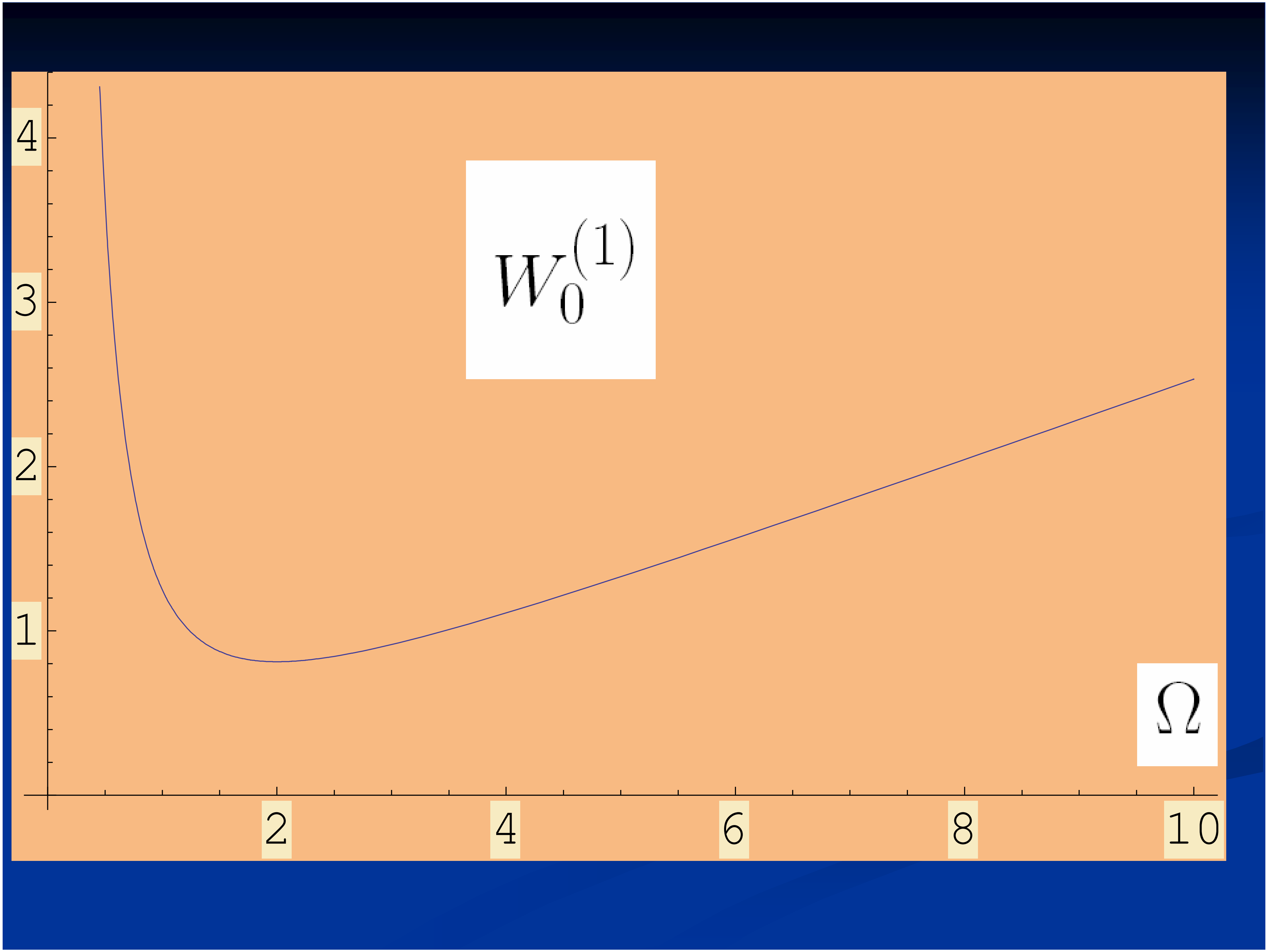
$$E_0^{(1)} = \frac{\omega}{2} + g\,\frac{3}{4\omega^2}$$

Identity

$$\equiv \frac{\Omega}{2}\sqrt{1+\frac{\omega^2-\Omega^2}{\Omega^2}} + g\,\frac{3}{4\Omega^2\sqrt{1+\frac{\omega^2-\Omega^2}{\Omega^2}}^{2}}$$

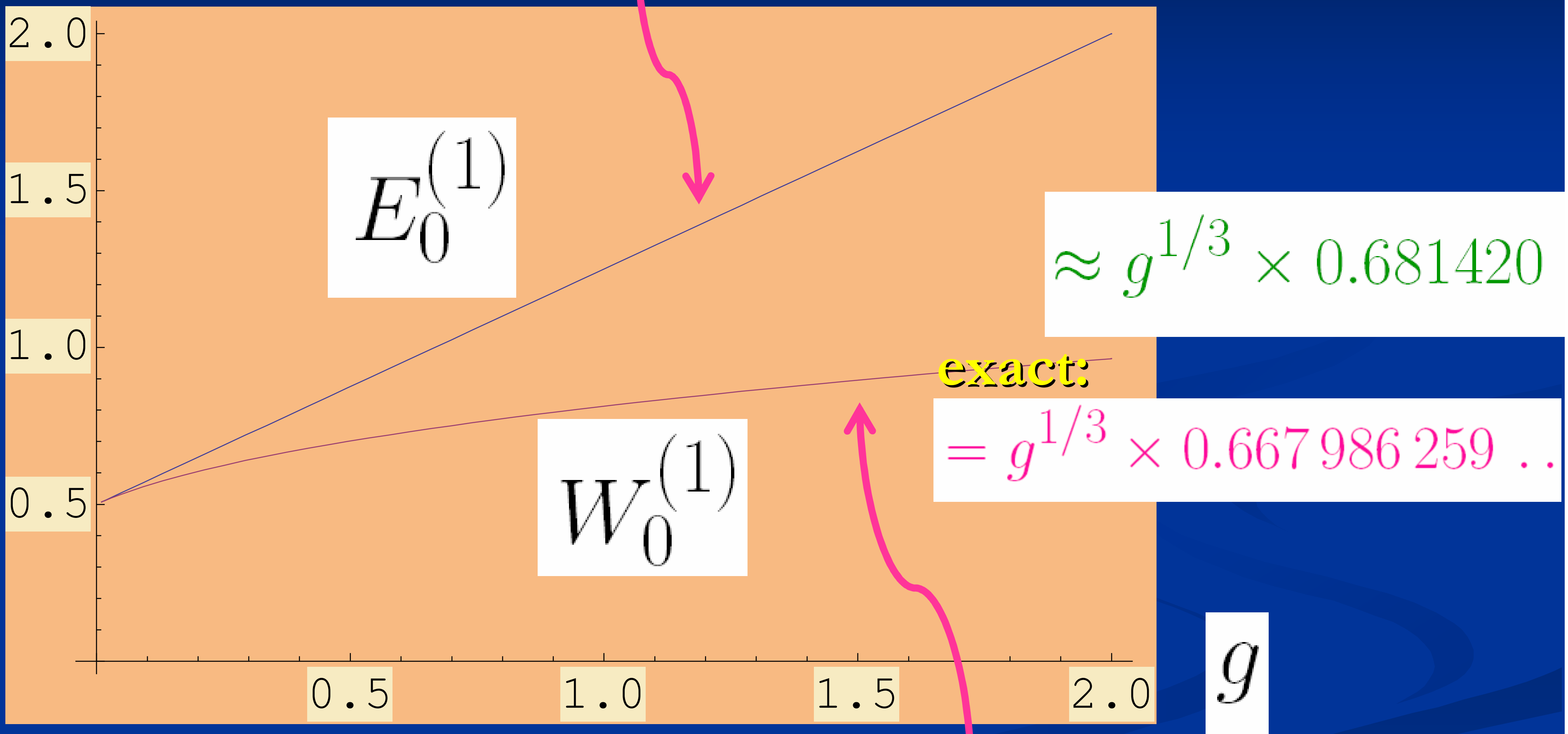
Expand to first order in: $\frac{\omega^2-\Omega^2}{\Omega^2}$

$$W_0^{(1)} \approx \frac{\Omega}{4} + \frac{\omega^2}{4\Omega} + g\,\frac{3}{4\Omega^2}$$



4
3
2
1
$W_0^{(1)}$
Ω
2
4
6
8
10

1 st order perturbation



1 st order variational perturbation

$$W_0^{(1)} \approx \frac{\Omega}{4} + \frac{\omega^2}{4\Omega} + g\,\frac{3}{4\Omega^2}$$

$$\omega = 1$$

Simple Strong-Coupling Limit:

$$\Omega \approx c g^{1/3}, \qquad E_0^{(1)} \approx g^{1/3}\left(\frac{c}{4} + \frac{3}{4c^2}\right)$$

Optimized at $c = 6^{1/3}$. Hence

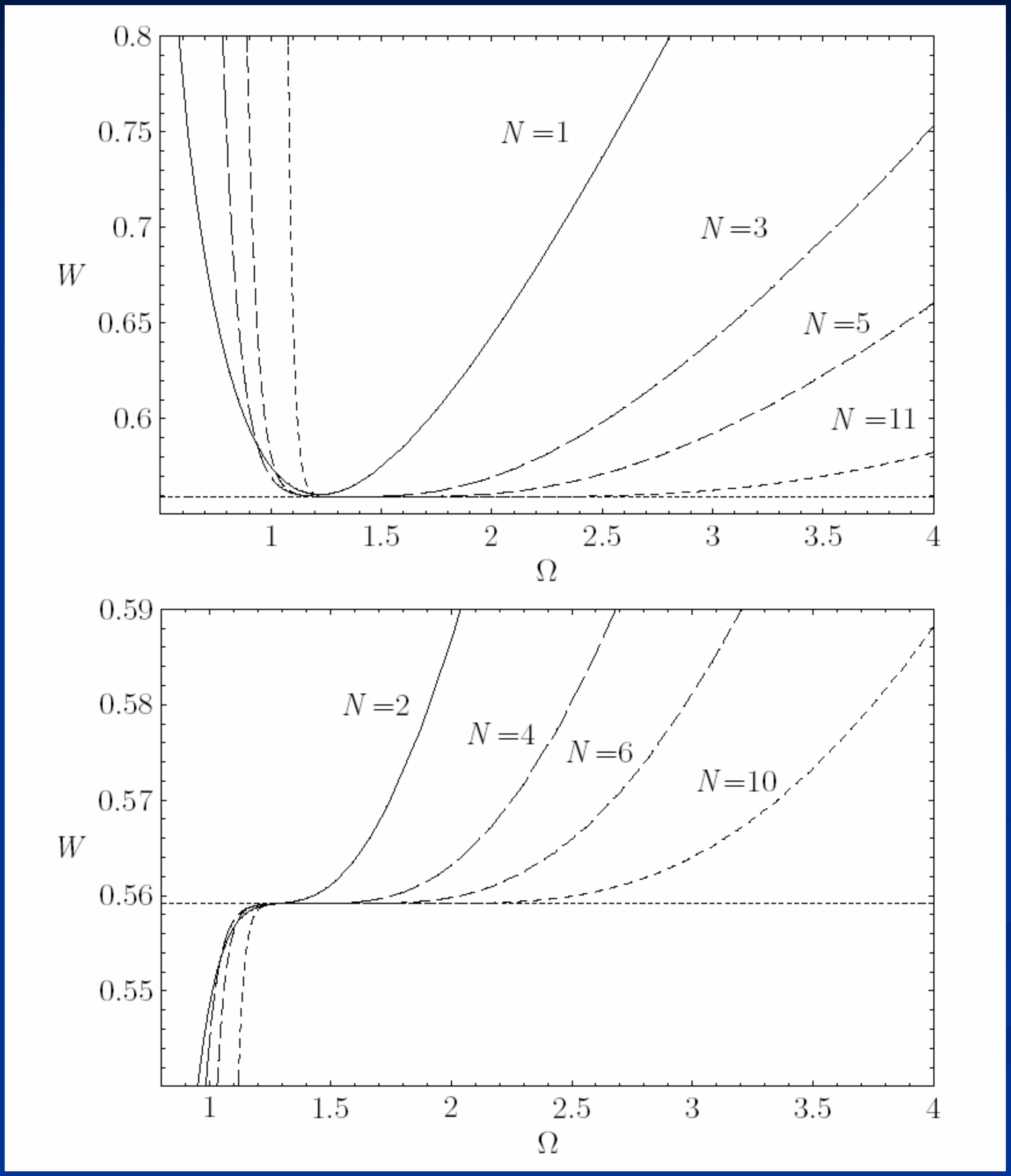
$$E_0^{(1)} \approx g^{1/3}\left(\frac{3}{4}\right)^{4/3} \approx g^{1/3} \times 0.681420$$

exact : $= g^{1/3} \times 0.667\,986\,259$

...

p	q	p/q	$2/q$
1	3	1/3	2/3

Higher Odd vs. Even Orders



up to 40 Digits:

PHYSICAL REVIEW LETTERS

VOLUME 75 | 9 OCTOBER 1995 | NUMBER 15

Convergent Strong-Coupling Expansions from Divergent Weak-Coupling Perturbation Theory

W. Janke[1,2] and H. Kleinert[2]

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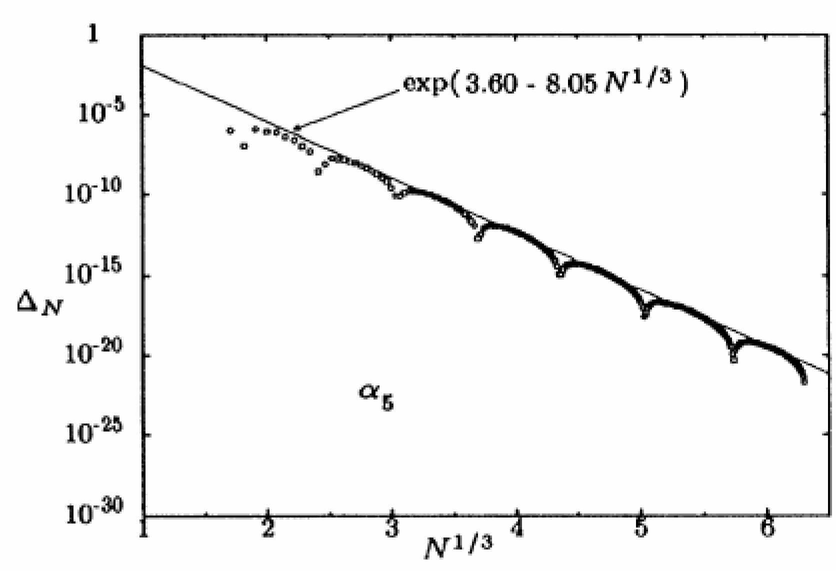
[2]*Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany*

Accuracy



Oscillations Related to Convergence Radius of SC-Expansion

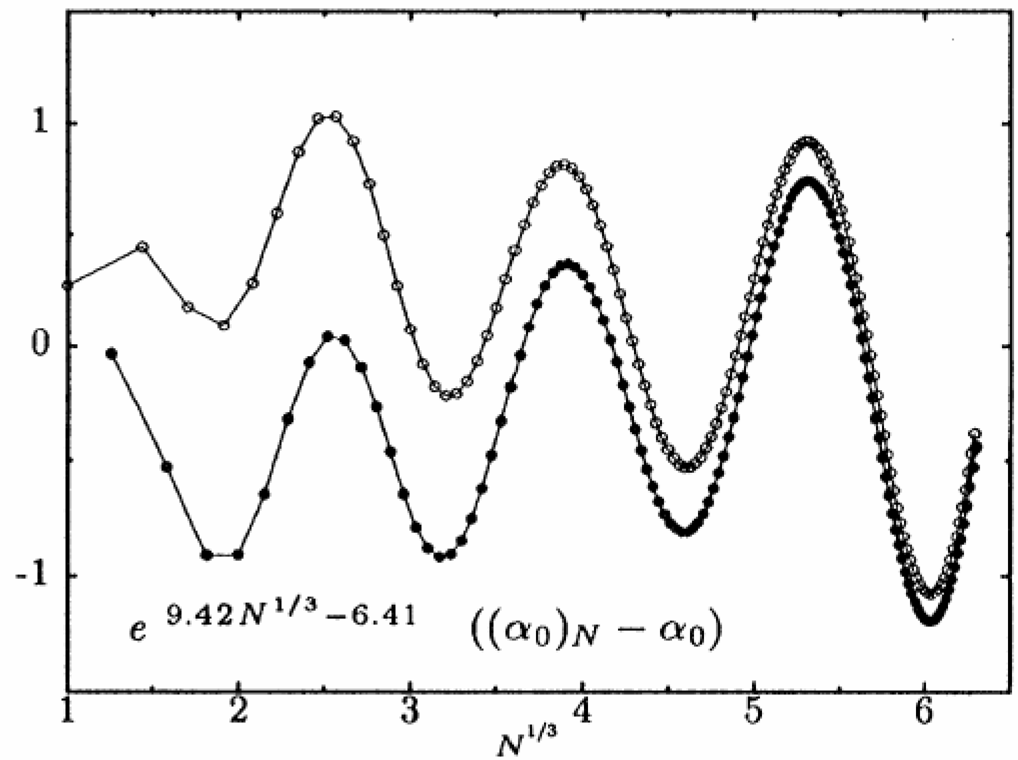


FIG. 2. Oscillatory behavior around the exponential approach to the limiting value of α_0.

W. Janke, H. Kleinert, PRL 75, 2787 (1995)

R. Guida, K. Konishi, H. Suzuki , Ann .Phys. 249, 109 (1996)

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LETTERS

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World record 62 Digits:

Upper and lower bounds of the ground state energy of anharmonic oscillators using renormalized inner projection

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VOLUME 77, NUMBER 14 | PHYSICAL REVIEW LETTERS | 30 SEPTEMBER 1996

Construction of the Strong Coupling Expansion for the Ground State Energy of the Quartic, Sextic, and Octic Anharmonic Oscillator via a Renormalized Strong Coupling Expansion

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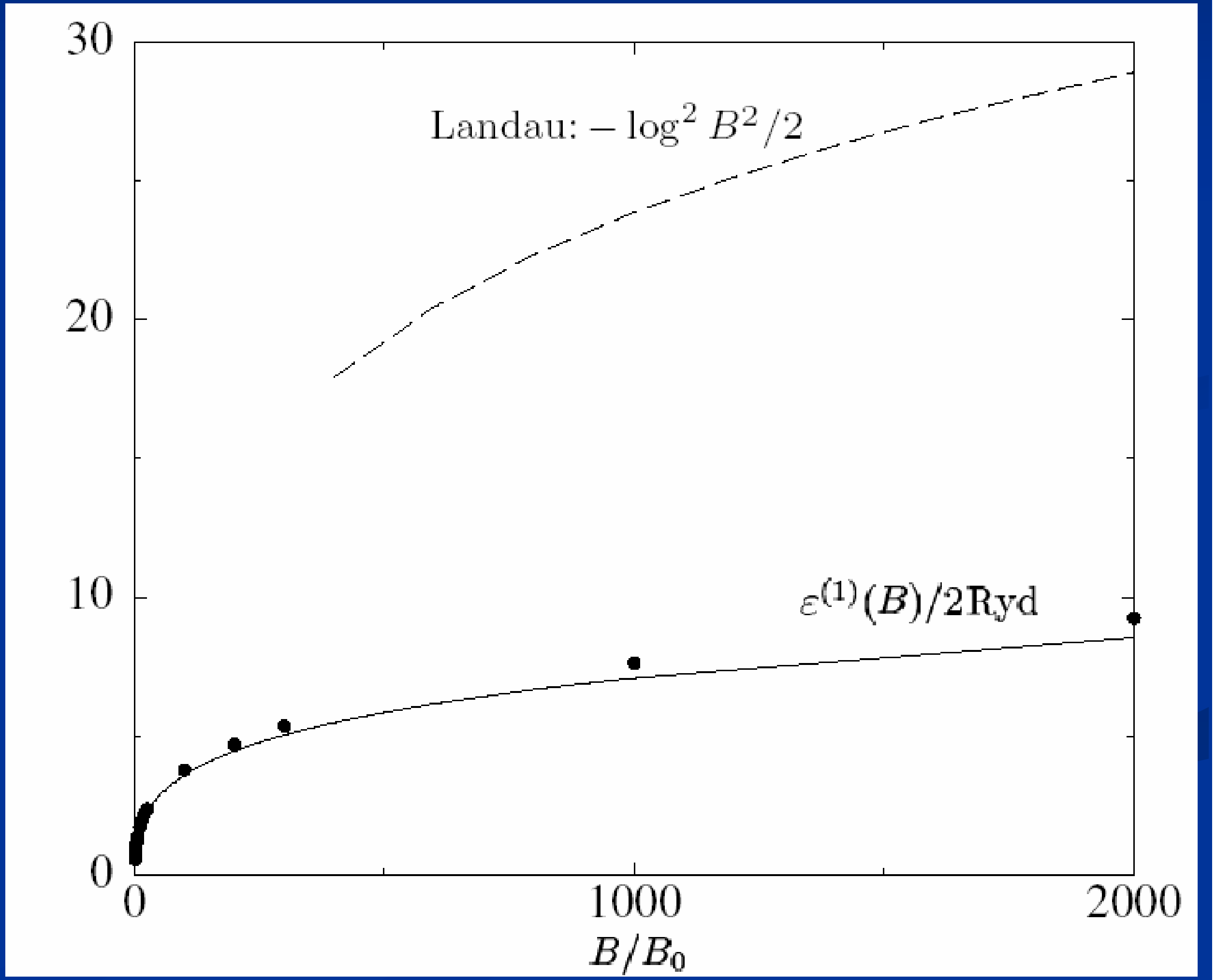
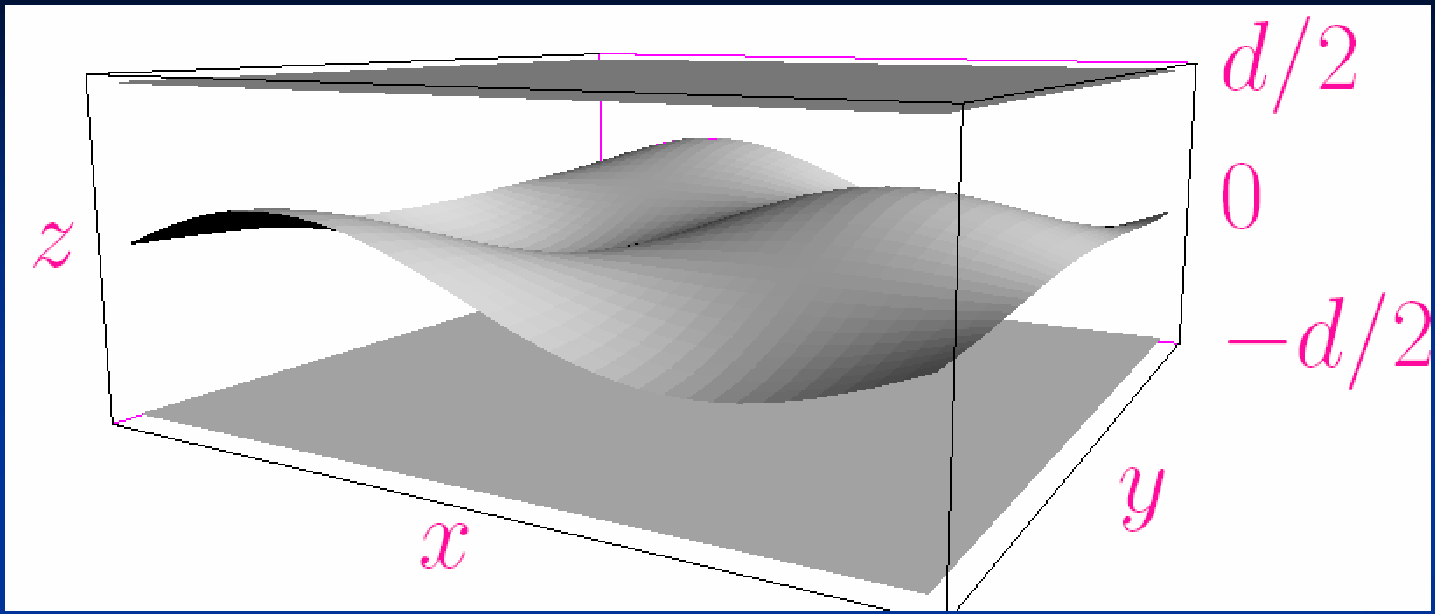
(Received 10 November 1995)

H-Atom in Strong Magnetic Field

Binding energy:



Membrane between Walls



- Harmonic bending energy:

$$E = \frac{1}{2}\kappa \int d^2x \left[\partial^2 \varphi(\mathbf{x})\right]^2$$

κ: elasticity constant

$\varphi(\mathbf{x})$: vertical displacement at $\mathbf{x} = (x, y)$

- Pressure law:

$$p = \alpha \frac{(k_B T)^2}{\kappa (d/2)^3}$$

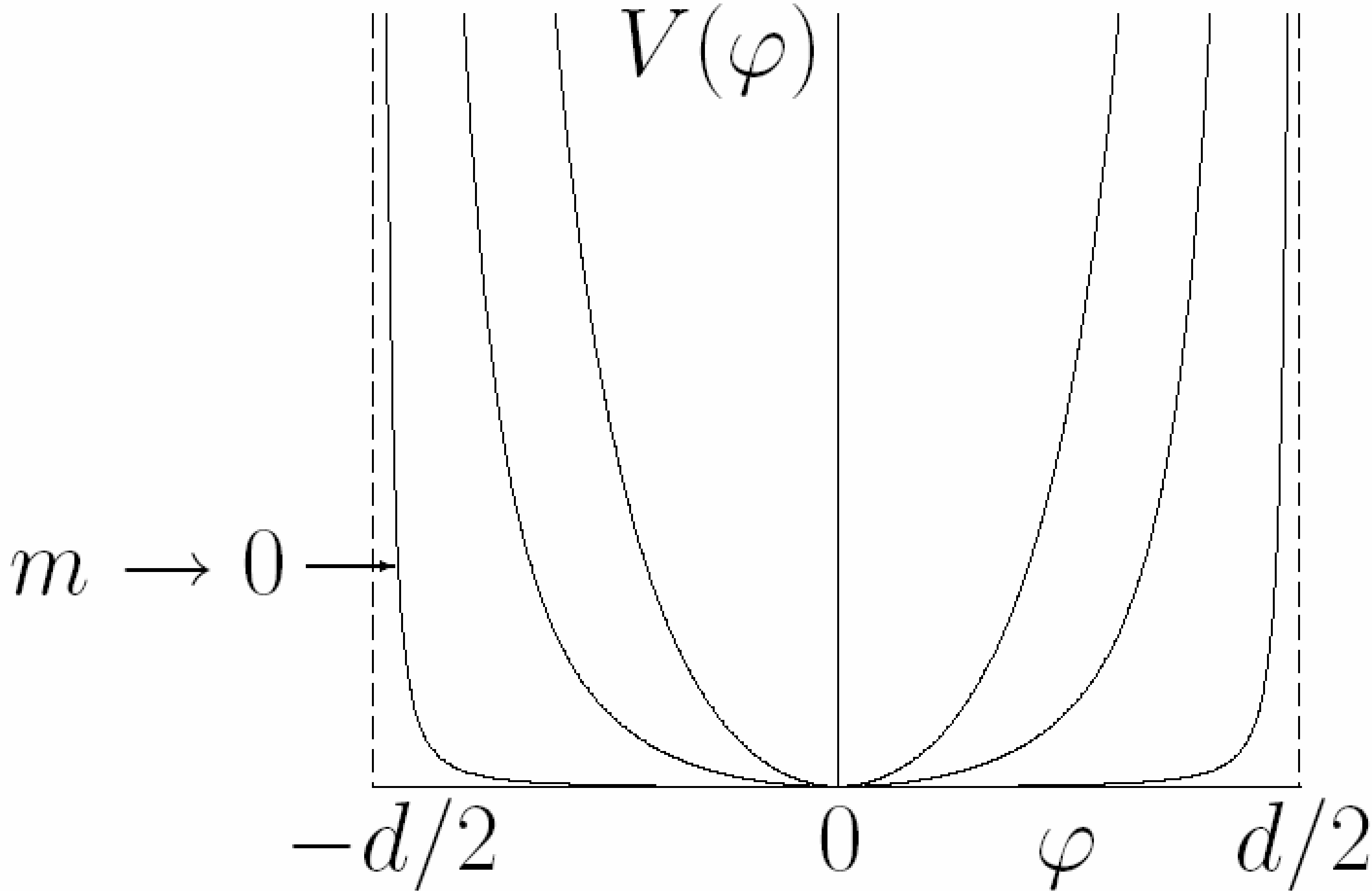
[Helfrich, Z. Naturforschung **A 33**, 305 (1978)]

- Partition function:

$$Z = \prod_{\mathbf{x}} \left[\int_{-d/2}^{+d/2} \frac{d\varphi(\mathbf{x})}{\sqrt{2\pi k_B T/\kappa}} \right] \times \exp\left\{ -\frac{\kappa}{2k_B T} \int d^2x \, [\partial^2 \varphi(\mathbf{x})]^2 \right\}$$

- Auxiliary potential restricting fluctuations:

$$V(\varphi) = m^4 \frac{d^2}{\pi^2} \tan^2\left(\frac{\pi\varphi}{d}\right)$$

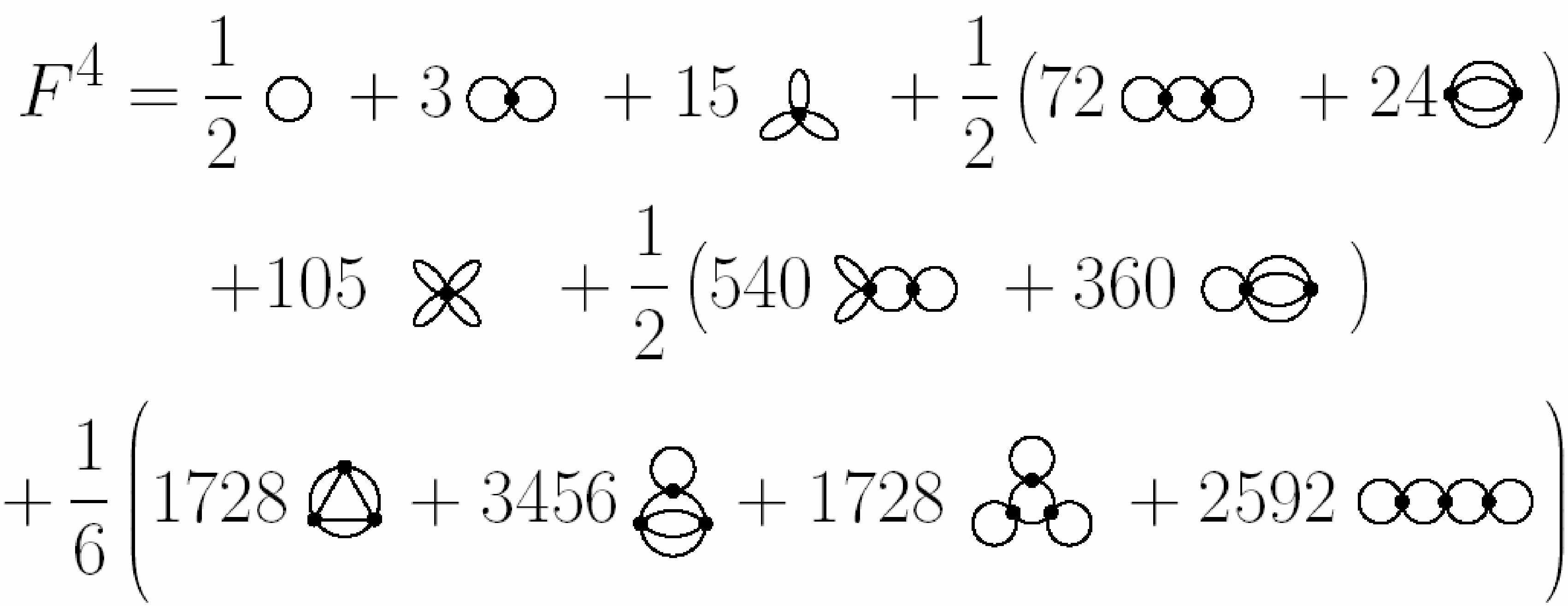


- Power expansion:

$$V(\varphi) = m^4\varphi^2 + m^4\frac{\pi^2}{d^2}\left\{\frac{2}{3}\varphi^4 + \frac{17}{45}\frac{\pi^2}{d^2}\varphi^6 + \frac{62}{315}\frac{\pi^4}{d^4}\varphi^8 + \dots\right\}$$

[H. Kleinert, Phys. Lett. A **257** , 269 (1999)

- Free energy:



- Weak-coupling series:

$$F^N = m^2 \left\{ a_0 + \sum_{n=1}^{N} a_n \left(\frac{\pi^2}{m^2 d^2} \right)^n \right\}$$

- Strong-coupling limit ($m \to 0$):

$$\alpha^{\text{th}} = 0.0797149$$

[Bachmann, Kleinert, Pelster, Phys. Lett. **A 261**, 127 (1999)]

- Monte-Carlo result:

$$\alpha^{\text{MC}} = 0.0798 \pm 0.0003$$

[Janke, Kleinert, Phys. Lett. **A 117**, 353 (1986)
Gompper, Kroll, Europhys. Lett. **9**, 59 (1989)]

Non-Borel Series

ELSEVIER

Physics Letters B 564 (2003) 111–114

www.elsevier.com/locate/npe

Tunnelling amplitudes from perturbation expansions

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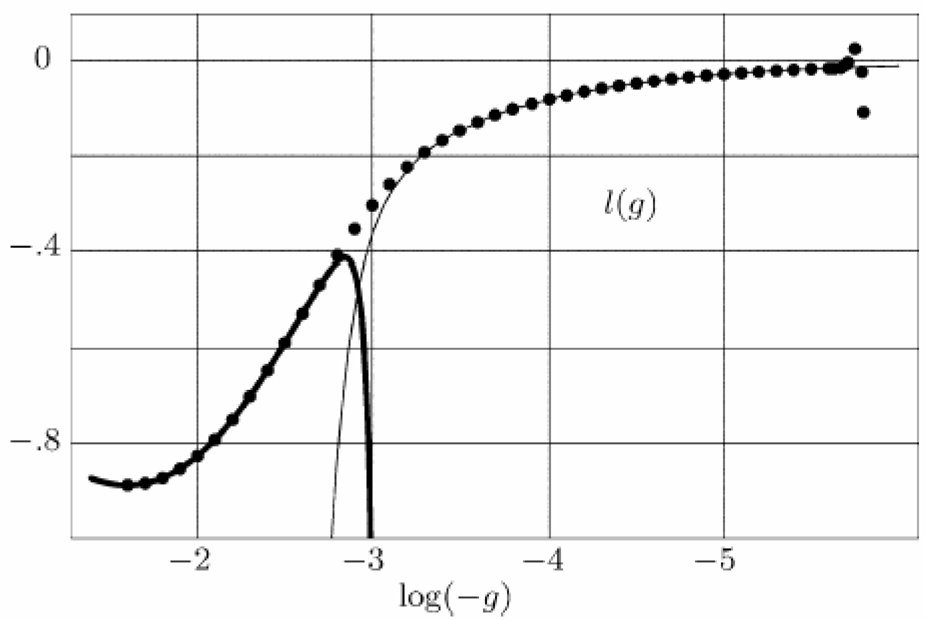

Fig. 2. Logarithm of the imaginary part of the ground state energy of the anharmonic oscillator with the essential singularity factored out for better visualization, $l(g) = \log[\sqrt{-\pi g/2}\, E_{0,\mathrm{var}}^{(64)}(g)] - 1/3g$,

Field Theoretic Variational Pert. Theory

- Weak-coupling series:

$$f_N(g) = \sum_{n=0}^{N} a_n \, g^n$$

- Rescaling:

$$f_N(g) = \kappa^p \sum_{n=0}^{N} a_n \left(\frac{g}{\kappa^q}\right)^n$$

- Now use square-root trick:

$$\kappa = \sqrt{K^2 + (\kappa^2 - K^2)} = K\sqrt{1 + g\,r}\,, \qquad r = \frac{\kappa^2/K^2 - 1}{g}$$

	p	q	p/q	$2/q$
anharmonic oscillator	1	3	1/3	2/3
ϕ^4-theory $(D = 4 - \epsilon)$	0	$2\epsilon/\omega$	0	ω/ϵ

PHYSICAL REVIEW D **68**, 065001 (2003)

Dependence of variational perturbation expansions on strong-coupling behavior: Inapplicability of δ expansion to field theory

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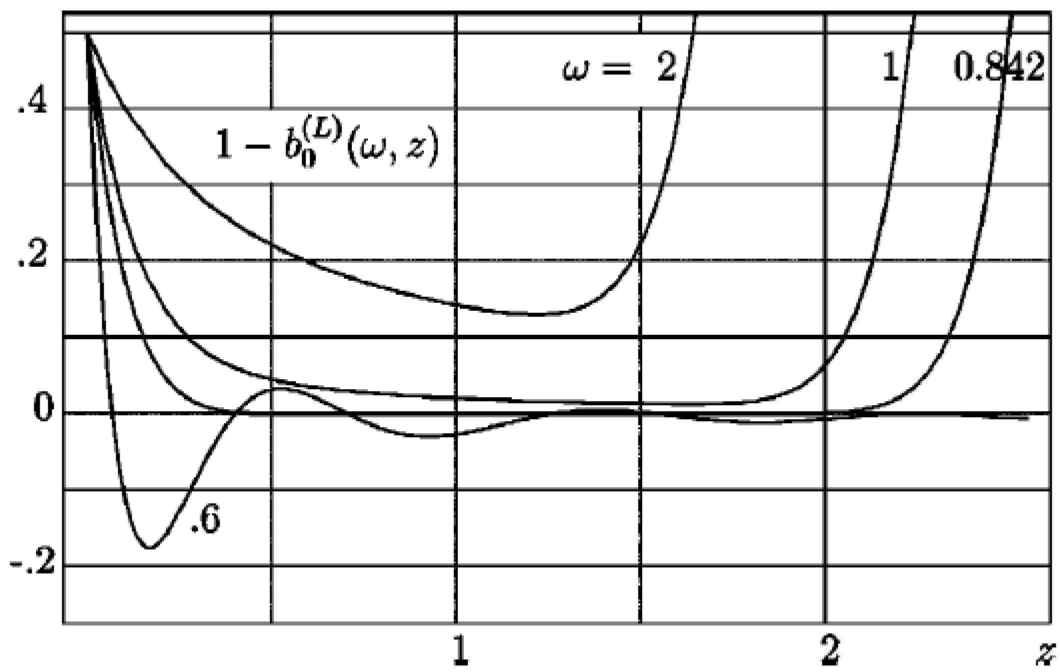
(Received 18 February 2003; revised manuscript received 12 May 2003; published 3 September 2003)



- Replacement of r, and $\kappa = 1$:

$$f_N(g,K) = \sum_{n=0}^{N} \sum_{k=0}^{N-n} a_n \binom{\frac{p-qn}{2}}{k} \left(K^{-2}-1\right)^k K^{p-qn} g^n$$

- Principle of minimal sensitivity:

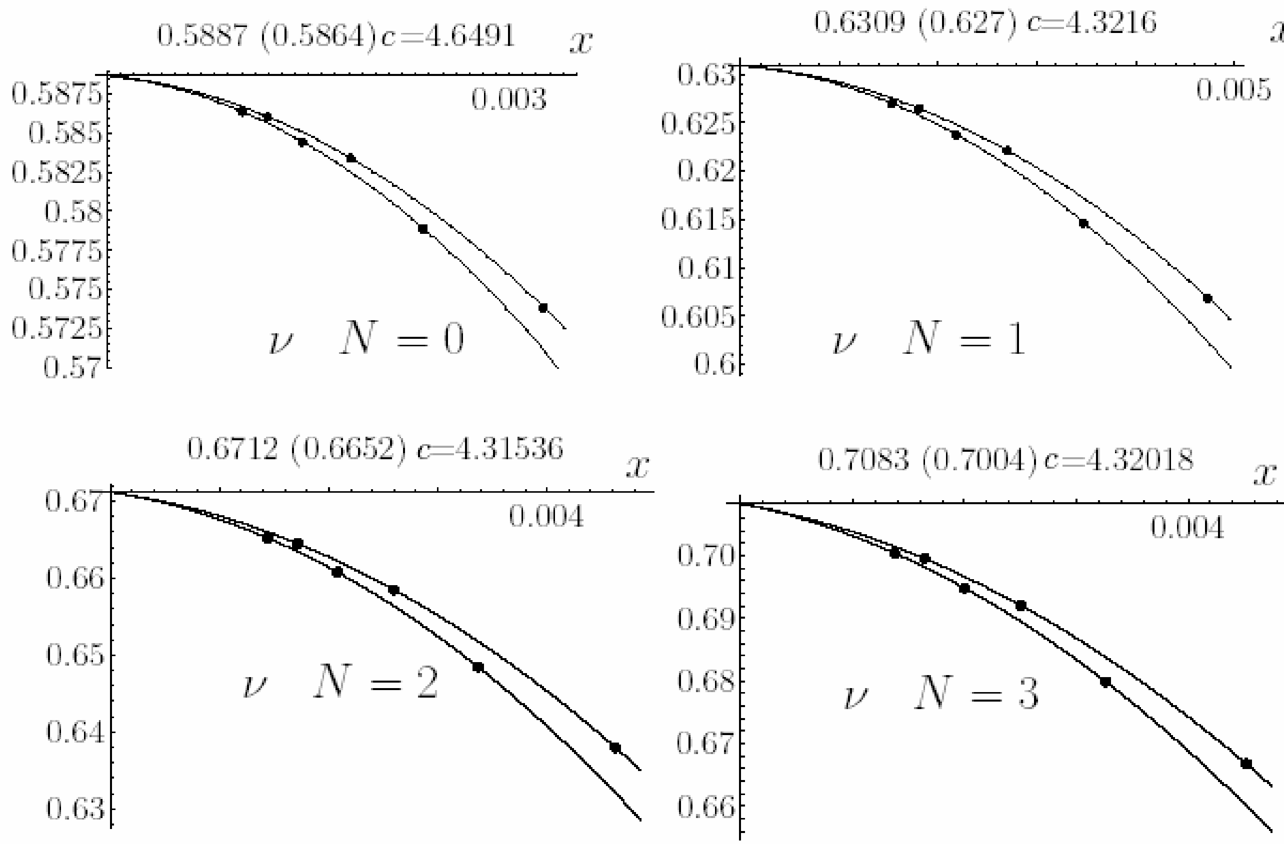
$$\frac{\partial}{\partial K} f_N(g,K) = 0 \quad \Rightarrow \quad K_N(g)$$

- Strong-coupling expansion:

$$K(g) = g^{\frac{1}{q}} \left\{ c_0 + c_1\, g^{-\frac{2}{q}} + c_2\, g^{-\frac{4}{q}} + \ldots \right\}$$

$$f(g) = g^{\frac{p}{q}} \left\{ b_0 + b_1\, g^{-\frac{2}{q}} + b_2\, g^{-\frac{4}{q}} + \ldots \right\}$$

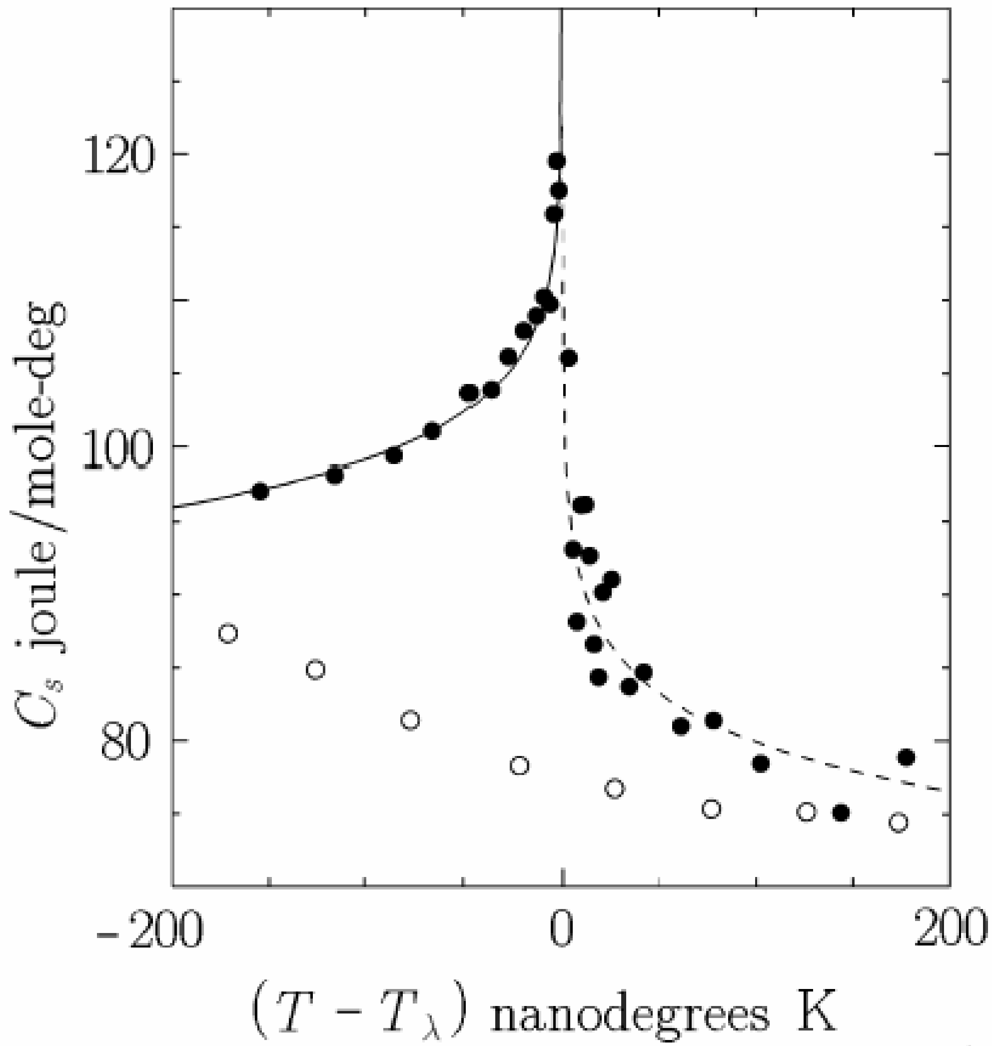
Examples



Strong-coupling values for the critical exponent $\nu^{-1}(x)$

$x(L) = e^{-cL^{1-\omega}}$

• Specific heat of superfluid helium:



Lipa, Swanson, Nissen, Chui, Israelson, PRL **76**, 944 (1996)

Beyond Hubbard-Stratonovich which is good only for large N

$$Z[j] = \mathcal{N} \int \mathcal{D}\phi e^{i \int d^4x \left\{ \frac{1}{2}(\partial\phi_a)^2 - \frac{m_0^2}{2}\phi_a^2 - \frac{g}{4}\left(\phi_a^2\right)^2 + j_\mu \phi_a \right\}}$$

$$= \mathcal{N} \int \mathcal{D}\phi \mathcal{D}\sigma e^{i \int d^4x \left\{ \frac{1}{2}\phi_a\left(-\partial^2 - m_0^2 - \sigma\right)\phi_a + \frac{1}{4g}\sigma^2 + j_a\phi_a \right\}}$$

$$= \mathcal{N} \int \mathcal{D}\sigma e^{i \int d^4x \left\{ \frac{1}{4g}\sigma^2 + iN\frac{\hbar}{2}\mathrm{Tr}\log\left(-\partial^2 - m_0^2 - \sigma\right) + \frac{i}{2} j \frac{i}{-\partial^2 - m_0^2 - \sigma} j \right\}}$$

$$\begin{aligned} \langle\phi_a\phi_b\phi_c\phi_d\rangle &\approx \langle\phi_a\phi_b\rangle\langle\phi_c\phi_d\rangle + \langle\phi_a\phi_c\rangle\langle\phi_b\phi_d\rangle + \langle\phi_a\phi_d\rangle\langle\phi_b\phi_c\rangle \\ &= \text{Hartree} + \text{Fock} + \text{Bogoliubov} \end{aligned}$$

Hubbard-Stratonovich misses two of these

Annals of Physics **266**, 135–161 (1998)
Article No. PH985789

Systematic Improvement of Hartree–Fock–Bogoliubov Approximation with Exponentially Fast Convergence from Variational Perturbation Theory

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Add and subtract to action:

$$\psi^\dagger \psi \rho + \psi \psi \Delta^* + \psi^\dagger \psi^\dagger \Delta$$

Include the adderd terms in free part,

the subtracted terms in the interaction.

Extremize in ρ and Δ, Δ^*.

If you want to know more, read my books