Critical exponents from a Landau-like approach

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Abstract

Landau's approach to continuous phase transitions provides an effective theory for the description around the critical point but falls short in correctly establishing non-trivial critical exponents. Using the example of the Mott-insulator to superfluid transition of the Bose-Hubbard model, we derive from the microscopic properties a Landau-like description not restricted by this limitation and correctly reproduce the best known value for the critical exponent β of the XY universality class.

Landau's approach

Continuous phase transitions are often described by **Landau's approach** [Lan69]: Assume that the thermodynamical potential Γ of a given system possesses the form

$$\Gamma = a_0 + a_2\psi^2 + a_4\psi^4 \,, \tag{1}$$

where the coefficients a_0, a_2, a_4 depend on a **control parameter** j, and the system adopts, for each fixed value of j, that value $\psi_{\min}$ of ψ for which the potential (1) takes on its minimum. If then a_4 is positive and thus guarantees stability, and if one may further neglect the dependence of a_4 on j, while a_2 crosses zero at some value j_c, being positive for $j < j_c$ and negative for $j > j_c$, one finds $\psi_{\min} = 0$ for $j < j_c$, whereas

$$\psi_{\min} = \left(\frac{-a_2}{2a_4}\right)^{1/2} \qquad \text{for} \quad j > j_c \,. \tag{2}$$

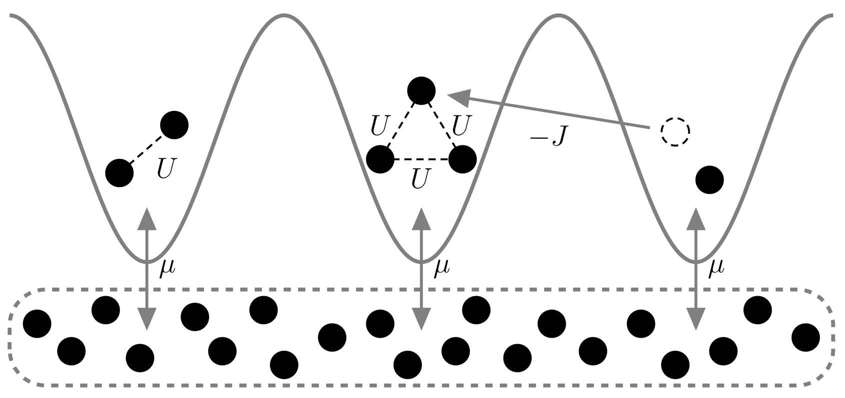
In particular, if a_2 varies linearly with j according to $a_2(j) = -\alpha\big(j - j_c\big)$ with $\alpha > 0$, one obtains

$$\psi_{\min} = \sqrt{\frac{\alpha}{2a_4}}(j - j_c)^{1/2} \qquad \text{for} \quad j > j_c \,. \tag{3}$$

Thus, $\psi_{\min}$ serves as an **order parameter** of the transition, emerging with the mean-field exponent $\beta = 1/2$ at the transition point j_c.

The Bose-Hubbard model

The Bose-Hubbard model is an archetypal description of Bose particles on a lattice which incorporates nearest neighbor tunneling as well as a repulsive on-site interaction and has the grand-canonical Hamiltonian



$$\widehat{H}_{\rm BH} = \frac{1}{2}\sum_i \widehat{n}_i(\widehat{n}_i - 1) - \mu/U\sum_i \widehat{n}_i - J/U\sum_{\langle i,j\rangle} \widehat{b}_i^\dagger\widehat{b}_j \,. \tag{4}$$

Derivation of the effective potential

We extend the Bose-Hubbard model by adding spatially homogeneous sources and drains, as expressed by the extended Hamiltonian

$$\widehat{H} = \frac{1}{2}\sum_i \widehat{n}_i(\widehat{n}_i - 1) - \mu/U\sum_i \widehat{n}_i - J/U\sum_{\langle i,j\rangle} \widehat{b}_i^\dagger\widehat{b}_j + \sum_i \eta\left(\widehat{b}_i^\dagger + \widehat{b}_i\right) \,. \tag{5}$$

Then the linear response

$$2\cdot\psi(\eta) := \frac{\partial\mathcal{E}}{\partial\eta} \tag{6}$$

of the intensive ground state energy $\mathcal{E} := \langle\widehat{H}\rangle_{\rm gs}/M$ with respect to the source strength η has the characteristic of an **order parameter** and the **Legendre transformation**

$$\Gamma\big(\mu/U, J/U, \psi\big) = \mathcal{E}\big(\mu/U, J/U, \eta(\psi)\big) - 2\psi\,\eta(\psi) \,, \tag{7}$$

allows us to derive an effective potential Γ as a function of ψ. The system then adopts, for each combination of fixed values of $(\mu/U, J/U)$, that value $\psi_{\min}$ for which the effective potential (7) takes on its minimum; in perfect analogy to Landau's approach.
To evaluate the effective potential we have expanded the intensive ground state energy

$$\mathcal{E}(\mu/U, J/U, \eta) = e_0(\mu/U, J/U) + \sum_{k=1}^{\infty} c_{2k}(\mu/U, J/U)\,\eta^{2k} \,. \tag{8}$$

Inserted into equation (7) the effective potential Γ then becomes

$$\Gamma = e_0 - \frac{1}{c_2}\psi^2 + \frac{c_4}{c_2^4}\psi^4 + \left(\frac{c_6}{c_2^6} - \frac{4c_4^2}{c_2^7}\right)\psi^6 + \mathcal{O}(\psi^8) \,. \tag{9}$$

Hypergeometric analytic continuation

The sought-after zero of the coefficient $a_2 := -1/c_2$ corresponds to the denominator's radius of convergence. This means that we have to combine our perturbation theoretical expansion of the coefficients c_{2k} with an analytic continuation. We have shown that **hypergeometric functions** are an excellent candidate for this task [SH17b]:

$$c_{2k} = \alpha_{2k}^{(0)} \cdot {}_2F_1\left(a, b; c; \frac{J/U}{(J/U)_c}\right) = \alpha_{2k}^{(0)} \sum_{\nu=0}^{\infty} \frac{(a)_\nu\,(b)_\nu}{\nu!\,(c)_\nu}\left(\frac{J/U}{(J/U)_c}\right)^{\nu} . \tag{10}$$

This, in particular, implies that the asymptotics of the coefficients are given by

$$c_{2k}(\mu/U, J/U) \sim \Big(J/U - \big(J/U\big)_c\Big)^{-\epsilon_{2k}(\mu/U)} \tag{11}$$

at the phase boundary with divergence exponents $\epsilon_{2k}(\mu/U)$.

Results

We have found that, in contrast to the simplistic form in equation (1), we are not entitled to neglect terms of order $\mathcal{O}(\psi^6)$, and have to consider the effective potential in the form

$$\Gamma = e_0 + a_2\psi^2 + a_4\psi^4 + a_6\psi^6 \,, \tag{12}$$

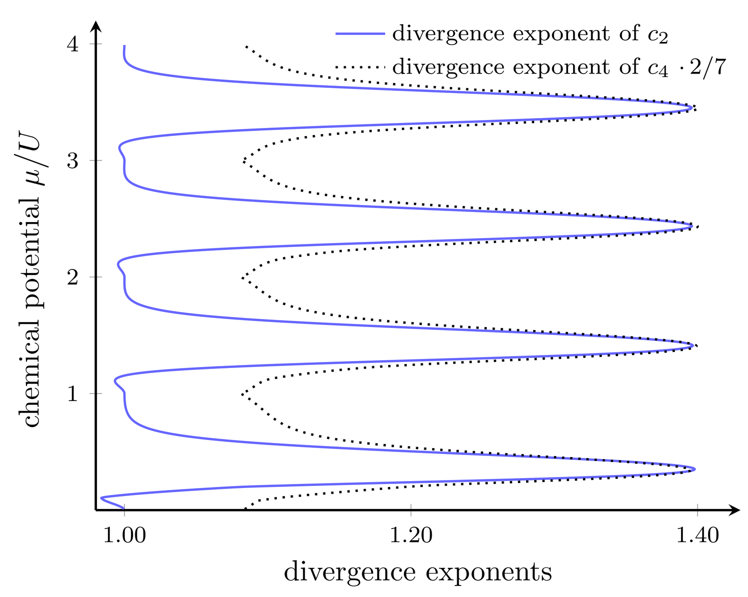
with its minimum given by

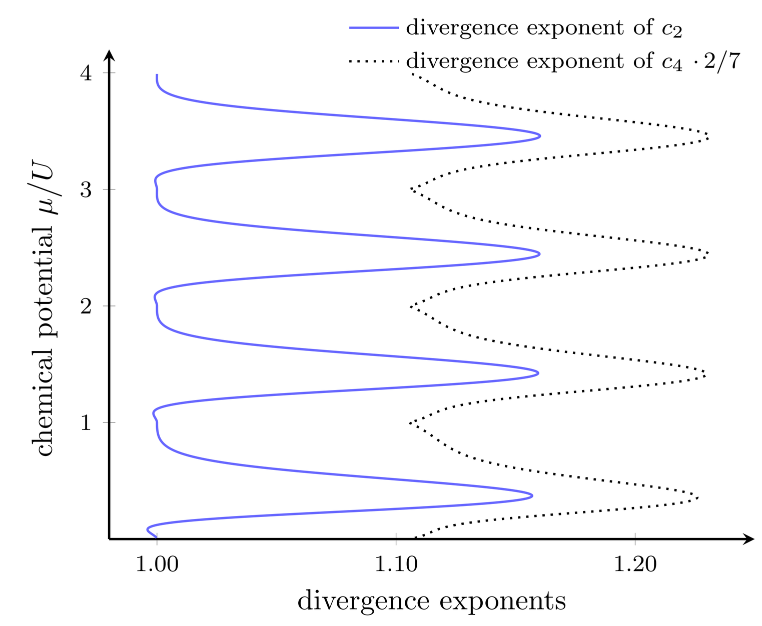
$$\psi_{\min}^2 = \frac{-a_4}{3a_6}\left(1 \pm \sqrt{1 - \frac{3a_2a_6}{a_4^2}}\right) . \tag{13}$$

For the truncation (12) to be bounded from below, we have to ask for a_6 to be positive. Under the validity of this assumption we can deduce that $\epsilon_6 \geq 2\epsilon_4 - \epsilon_2$ [SH17a]. In case, this is indeed an equality the exponent can be written as

$$\beta = \frac{\epsilon_4 - 3\epsilon_2}{2} \tag{14}$$

To check this premise, we have to study the coefficient $a_6 = \frac{c_6}{c_2^6} - \frac{4c_4^2}{c_2^7}$ in detail. As unfortunately, we lack reliable data for the coefficient c_6 we are restricted to the investigation of the term c_4^2/c_2^7. The results for the two-dimensional Bose-Hubbard (left) as well as for comparison the three-dimensional Bose-Hubbard model (right), which is above the critical dimension, are displayed below.





For the two-dimensional Bose-Hubbard model only we find the intriguing equality

$$\epsilon_4 = \frac{7}{2}\epsilon_2 \qquad \text{at the tips of the lobes} \,, \tag{15}$$

which inserted into relation (14) yields the simpler formula

$$\beta = \frac{\epsilon_2}{4} \tag{16}$$

for the critical exponent β at the multicritical tips of the lobes. This enables us to obtain the following estimates to the critical exponent β and compare them to the best known estimate $\beta = 0.3485(2)$ for the three-dimensional XY universality class.

lobe index g	β	relative deviation
1	0.3475	- 0.30%
2	0.3483	- 0.06%
3	0.3485	0.00%
4	0.3489	0.12%

Literature

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