Improving Ginzburg-Landau Theory for Bosons in Optical Lattices via Degenerate Perturbation Theory

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Abstract

Bosons in an optical lattice yield a paradigmatic quantum phase transition between a Mott insulator and a superfluid. Recently, a Ginzburg-Landau theory for the underlying Bose-Hubbard model has been developed, which allows to determine the location of this quantum phase transition quite accurately [1-3]. Here we extend the validity range of this Ginzburg-Landau theory with the help of a degenerate perturbation theory. This allows to study also harmonically confined optical lattices, where a wedding cake structure of insulating Mott shells with superfluid regions between the Mott shells emerge [4].

Brillouin-Wigner Perturbation Theory

We assume that the Hamiltonian decomposes according to $\hat{H} = \hat{H}^{(0)} + \lambda\hat{V}$, with λ being small and $\hat{H}^{(0)}$ having known eigenvalues and eigenfunctions: $\hat{H}^{(0)} | \Psi_n^{(0)} \rangle = E_n^{(0)} \Psi_n^{(0)}$. We split the underlying Hilbert space into two parts, each one projecting into different subspaces

$$\hat{Q} + \hat{P} = \mathbb{1}\,.$$

The projection operators are chosen in such a way to grant idempotency and that $\hat{H}^{(0)}$ commutes with $\hat{P}$

$$\hat{P}_n = | \Psi_n^{(0)} \rangle \langle \Psi_n^{(0)} |\,, \quad \hat{P} = \sum_{k \epsilon N} \hat{P}_k\,,$$

where we define $\tilde{N}$ as the complement of N. This allows us to rewrite the Schrödinger equation without a dependency on $\hat{Q}$

$$\hat{P}\hat{H}_{\text{eff}}\hat{P} | \Psi_n \rangle = E_n \hat{P} | \Psi_n \rangle\,,$$

where we introduce the effective Hamiltonian $\hat{H}_{\text{eff}}$

$$\hat{H}_{\text{eff}} = \hat{H} + \lambda^2 \hat{V}\hat{Q}\left(E_n - \hat{Q}\hat{H}\hat{Q}\right)^{-1}\hat{Q}\hat{V}\,.$$

We expand the resolvent into a Taylor series with respect to λ with the help of a geometric series

$$\hat{R}(E_n) = \left(E_n - \hat{Q}\hat{H}\hat{Q}\right)^{-1} = \left(E_n - \hat{Q}\hat{H}^{(0)}\hat{Q}\right)^{-1} \sum_{s=0}^{\infty} \left[\lambda \hat{Q}\hat{V}\hat{Q}\left(E_n - \hat{Q}\hat{H}^{(0)}\hat{Q}\right)^{-1}\right]^s\,.$$

With this, we get the effective Hamiltonian up to the fourth order in λ

$$\begin{aligned}\hat{H}_{\text{eff}} =& \hat{H}^{(0)} + \lambda\hat{V} + \lambda^2 \hat{V}\hat{Q}\hat{R}^{(0)}(E_n)\hat{Q}\hat{V} + \lambda^3 \hat{V}\hat{Q}\hat{R}^{(0)}(E_n)\hat{Q}\hat{V}\hat{Q}\hat{R}^{(0)}(E_n)\hat{Q}\hat{V} \\ &+ \lambda^4 \hat{V}\hat{Q}\hat{R}^{(0)}(E_n)\hat{Q}\hat{V}\hat{Q}\hat{R}^{(0)}(E_n)\hat{Q}\hat{V}\hat{Q}\hat{R}^{(0)}(E_n)\hat{Q}\hat{V} + \ldots\,.\end{aligned}$$

For one state we get the result of Brillouin-Wigner perturbation theory

$$E_n = E_n^{(0)} + \lambda V_{n,n} + \lambda^2 \sum_{l\epsilon\tilde{N}} \frac{V_{n,l}V_{l,n}}{E_n - E_l^{(0)}} + \lambda^3 \sum_{l,l'\epsilon\tilde{N}} \frac{V_{n,l}V_{l,l'}V_{l',n}}{\left(E_n - E_l^{(0)}\right)\left(E_n - E_{l'}^{(0)}\right)} + \lambda^4 \sum_{l,l',l''\epsilon\tilde{N}} \frac{V_{n,l}V_{l,l'}V_{l',l''}V_{l'',n}}{\left(E_n - E_l^{(0)}\right)\left(E_n - E_{l'}^{(0)}\right)\left(E_n - E_{l''}^{(0)}\right)} + \ldots\,.$$

Out of this we obtain the energy correction terms of the Rayleigh-Schrödinger perturbation theory by performing the Taylor expansion

$$E_n = \sum_\sigma \lambda^\sigma E_n^{(\sigma)}$$

with respect to λ, yielding

$$\begin{aligned}E_n =& E_n^{(0)} + \lambda V_{n,n} + \lambda^2 \sum_{l\neq n} \frac{V_{n,l}V_{l,n}}{E_n^{(0)} - E_l^{(0)}} + \lambda^3 \left[\sum_{l,l'\neq n} \frac{V_{n,l}V_{l,l'}V_{l',n}}{\left(E_n^{(0)} - E_l^{(0)}\right)\left(E_n^{(0)} - E_{l'}^{(0)}\right)} - \sum_{l\neq n} \frac{V_{n,l}V_{l,n}V_{n,n}}{\left(E_n^{(0)} - E_l^{(0)}\right)^2}\right] + \lambda^4 \left\{\sum_{l,l'\neq n} \frac{V_{n,l}V_{l,l'}V_{l',n}V_{n,n}\left(2E_n^{(0)} - E_l^{(0)} - E_{l'}^{(0)}\right)}{-\left(E_n^{(0)} - E_l^{(0)}\right)^2\left(E_n^{(0)} - E_{l'}^{(0)}\right)^2}\right. \\ &\left. + \sum_{l,l',l''\neq n} \frac{V_{n,l}V_{l,l'}V_{l',l''}V_{l'',n}}{\left(E_n^{(0)} - E_l^{(0)}\right)\left(E_n^{(0)} - E_{l'}^{(0)}\right)\left(E_n^{(0)} - E_{l''}^{(0)}\right)} + \sum_{l\neq n} \frac{V_{n,l}V_{l,n}}{E_n^{(0)} - E_l^{(0)}} \left[\left(\frac{V_{n,n}}{E_n^{(0)} - E_l^{(0)}}\right)^2 - \frac{V_{n,l}V_{l,n}}{\left(E_n^{(0)} - E_l^{(0)}\right)^2}\right]\right\} + \ldots\,.\end{aligned}$$

For two states we obtain

$$\text{Det}\begin{pmatrix} H_{\text{eff},n,n} - E_n & H_{\text{eff},n,n'} \\ H_{\text{eff},n',n} & H_{\text{eff},n',n'} - E_n \end{pmatrix} = 0\,.$$

General Setting and Graphical Approach

We consider the setting of the Bose Hubbard Hamiltonian in mean field [5], namely

$$\hat{H}^{(0)} = \lambda J z \Psi^*\Psi + \frac{1}{2}U\hat{n}\left(\hat{n} - 1\right) - \mu\hat{n}\,.$$

Here, J is the hopping energy, z is the number of nearest neighbours, U is the interaction energy and μ is the chemical potential. Ψ is the order parameter, so that $\Psi = 0$ in the Mott phase, whereas $\Psi \neq 0$ in the superfluid phase. $\hat{V}$ is given as

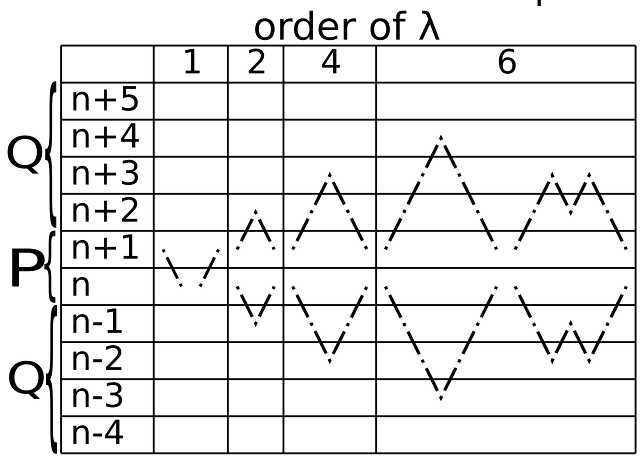
$$\hat{V} = -Jz\left(\Psi^*\hat{a} + \Psi\hat{a}^\dagger\right)\,,$$

where $\hat{a}$ and $\hat{a}^\dagger$ are the corresponding bosonic annihilation and creation operator. The graphical approach for the matrix elements translates into a formula with:

$S\left(\eta\right) = E_n - E_\eta^{(0)}$, graph starts in state η

$L_A\left(\nu\right) = \lambda J z \Psi \dfrac{\sqrt{\nu + 1}}{E_n - E_\nu^{(0)}}$, ascending line starting in ν

$L_D\left(\nu\right) = \lambda J z \Psi^* \dfrac{\sqrt{\nu}}{E_n - E_\nu^{(0)}}$, descending line starting in ν



Linear Approximation at Degeneracy n and $n+1$ [4]

We calculate the determinant of the two-state matrix with the effective Hamiltonian up to first order in λ

$$\text{Det}\begin{pmatrix} E_n^{(0)} - E_n & \lambda J z \Psi^* \sqrt{n+1} \\ \lambda J z \Psi \sqrt{n+1} & E_{n+1}^{(0)} - E_n \end{pmatrix} = 0\,.$$

This gives us the energy eigenvalues, from which we get the order parameter by differentiating with respect to Ψ^*, i. e. $\partial E_n / \partial \Psi^* = 0$

$$\Psi^*\Psi = \frac{n+1}{4} - \frac{\left(\mu - Un\right)^2}{4\lambda^2 J^2 z^2 \left(n+1\right)}\,. \tag{1}$$

With $\Psi^*\Psi = 0$, we get

$$\frac{Jz}{U} = \frac{\frac{\mu}{U} - n}{\lambda\left(n+1\right)}\,, \tag{2}$$

so that $\frac{Jz}{U}$ is a linear function of $\frac{\mu}{U}$, which represents a good approximation near the degenerate point of the lobes n and $n+1$.

Condensate Density $\Psi^*\Psi$ and Phase Boundary

To get the condensate density, we take the two-state matrix and go up to second order in λ

$$\text{Det}\begin{pmatrix} E_n^{(0)} - E_n + \lambda^2 \frac{J^2 z^2 \Psi^*\Psi n}{E_n - E_{n-1}^{(0)}} & -\lambda J z \Psi^* \sqrt{n+1} \\ -\lambda J z \Psi \sqrt{n+1} & E_{n+1}^{(0)} - E_n + \lambda^2 \frac{J^2 z^2 \Psi^*\Psi (n+2)}{E_n - E_{n+2}^{(0)}} \end{pmatrix} = 0\,.$$

We can neglect all orders in λ higher than 2 and achieve

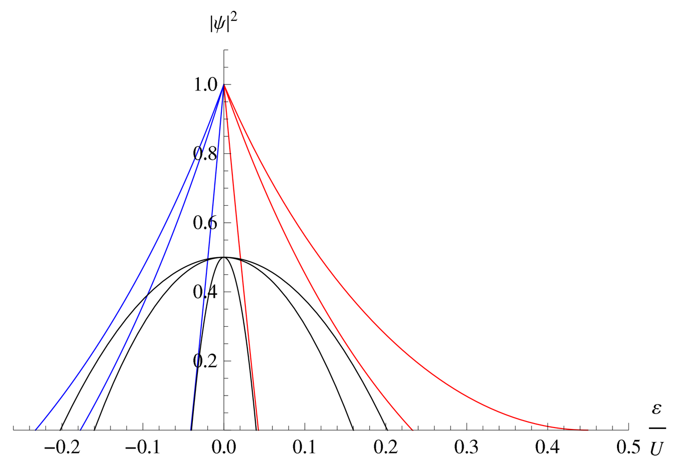
$$\left(E_n - E_n^{(0)}\right)\left(E_n - E_{n+1}^{(0)}\right) - \lambda^2 \left[\left(E_n - E_n^{(0)}\right)\frac{J^2 z^2 \Psi^*\Psi\left(n+2\right)}{E_n - E_{n+2}^{(0)}} + \left(E_n - E_{n+1}^{(0)}\right)\frac{J^2 z^2 \Psi^*\Psi n}{E_n - E_{n-1}^{(0)}} - \lambda^2 J^2 z^2 \Psi\Psi^*\left(n+1\right)\right] = 0\,.$$

Performing the partial derivative with respect to Ψ^*, dividing by Ψ and solving with respect to $\Psi^*\Psi$ in leading order in lambda gives us the condensate density. Thus we set $E_n = E_n^{(0)}$ for the n-Lobe and get

$$\Psi^*\Psi = \frac{\left(U + 2nU - 2\mu\right)\left[n^2U^2 - \left(Jz\lambda - \mu\right)\left(U + \mu\right) - nU\left(U + 2\mu\right)\right]}{2Jz\lambda\left[\left(-1 - 3n + n^2\right)U^2 + \left(3 - 2n\right)U\mu + \mu^2\right]}\,. \tag{3}$$

An equivalent formula can be found for $E_n = E_{n+1}^{(0)}$ for the $n+1$-Lobe.

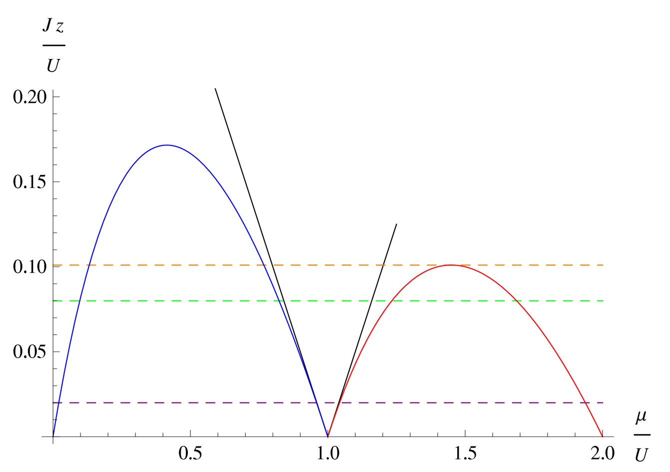
For the degenerate case that $E_n^{(0)} = E_{n+1}^{(0)}$ we have $\mu = Un$. To get the neighbourhood of the degeneracy as well, we put $\mu = Un + \varepsilon$ into the equation above. The black graphs origin from the formula (1), while the blue and red graphs origin from the formula (3) with $n = 1$. The graphs are plotted for $J = 0.101$, 0.08, 0.02 from top to bottom.



For the phase boundary, we set (3) equal to zero and solve it with respect to $\frac{Jz}{U}$

$$\frac{Jz}{U} = \frac{n - n^2 - \frac{\mu}{U} + 2n\frac{\mu}{U} - \left(\frac{\mu}{U}\right)^2}{\left(1 + \frac{\mu}{U}\right)\lambda}\,. \tag{4}$$

The black graph origins from equation (2), while the blue ($E_n = E_n^{(0)}$) and red ($E_n = E_{n+1}^{(0)}$) graphs origin from equation (4). The blue and red phase boundaries coincide with the mean-field result in [5].



Outlook

- taking higher order corrections into account
- going from Mean-Field Theory to Landau Theory
- getting the excitation spectra for the whole lobe [6]
- adding the impact of a trap to the calculations

References

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