Improving Mean-Field 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 [1-4]. Here we extend the validity range of the corresponding mean-field theory [5] 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 [6, 7].

Brillouin-Wigner Perturbation Theory

- Starting point: $\hat{H} = \hat{H}^{(0)} + \lambda\hat{V}$
- Two-state approach [8]:
- Operator $\hat{P}$ projects into two-dimensional subspace $\mathcal{H}_P = \{|n\rangle, |n+1\rangle\}$
- Effective Hamiltonian in subspace $\mathcal{H}_P$:

$$\hat{H}_{\text{eff}} = \hat{H}^{(0)} + \lambda\hat{V} + \lambda^2 \sum_{l\epsilon\bar{N}} \frac{\hat{V}|l\rangle\langle l|\hat{V}}{E_n - E_l^{(0)}} + \lambda^3 \sum_{l,l'\epsilon\bar{N}} \frac{\hat{V}|l\rangle\langle l|\hat{V}|l'\rangle\langle l'|\hat{V}}{\left(E_n - E_l^{(0)}\right)\left(E_n - E_{l'}^{(0)}\right)} + \ldots$$

- Perturbed energy eigenvalue E_n defined by:

$$\text{Det}\begin{pmatrix} \langle n|\hat{H}_{\text{eff}}|n\rangle - E_n & \langle n|\hat{H}_{\text{eff}}|n+1\rangle \\ \langle n+1|\hat{H}_{\text{eff}}|n\rangle & \langle n+1|\hat{H}_{\text{eff}}|n+1\rangle - E_n \end{pmatrix} = 0$$

- Unperturbed energy in mean field [5] and perturbation theory:

$$E_n^{(0)} = \frac{1}{2}Un(n-1) - \mu n \qquad \mathcal{E}_n^{(0)} = \frac{1}{2}Un(n-1) - \mu n + \lambda Jz\Psi^*\Psi$$

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

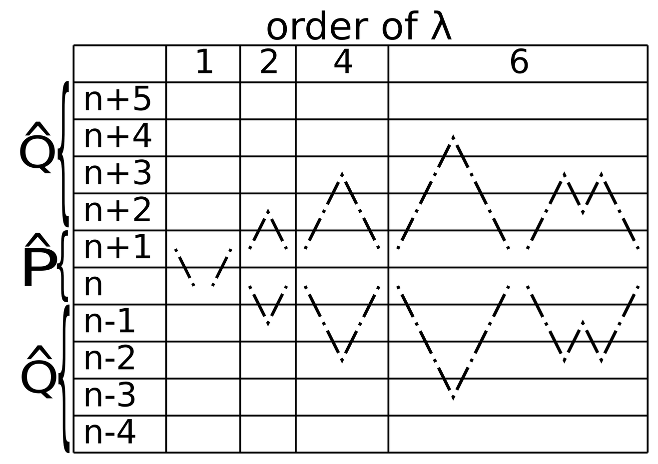
$\Psi = 0 \mathrel{\hat{=}}$ Mott phase, $\Psi \neq 0 \mathrel{\hat{=}}$ superfluid phase

- Graphical approach with $\hat{Q} = 1 - \hat{P}$:

$S(\eta) = E_n - \mathcal{E}_\eta^{(0)}$, graph starts in state η

$L_A(\nu) = \lambda Jz\Psi\frac{\sqrt{\nu+1}}{E_n - \mathcal{E}_\nu^{(0)}}$, ascending line starting in ν

$L_D(\nu) = \lambda Jz\Psi^*\frac{\sqrt{\nu}}{E_n - \mathcal{E}_\nu^{(0)}}$, descending line starting in ν



Linear Approximation at Degeneracy n and $n+1$ [7]

- Determinant of two-state matrix with effective Hamiltonian up to first order in λ:

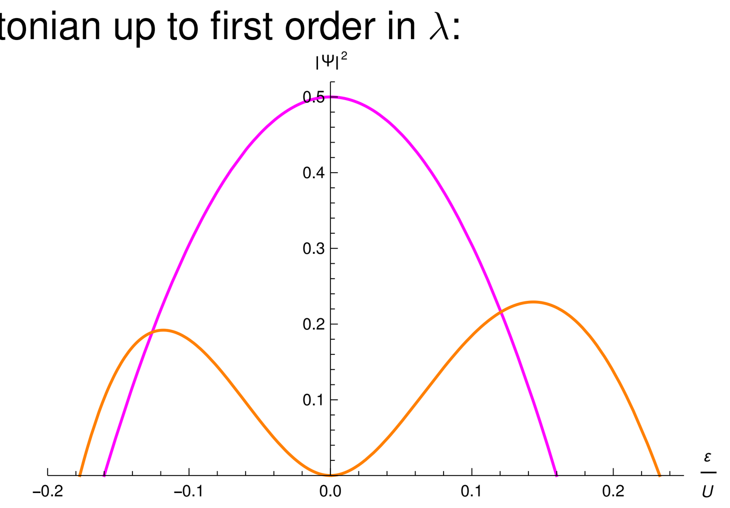
$$\text{Det}\begin{pmatrix} \mathcal{E}_n^{(0)} - E_n & \lambda Jz\Psi^*\sqrt{n+1} \\ \lambda Jz\Psi\sqrt{n+1} & \mathcal{E}_{n+1}^{(0)} - E_n \end{pmatrix} = 0$$

- Order parameter determined from $\partial E_n/\partial\Psi^* = 0$:

$$\Psi^*\Psi = \frac{n+1}{4} - \frac{(\mu - Un)^2}{4\lambda^2 J^2 z^2 (n+1)} \qquad (1)$$

- Phase boundary follows from $\Psi^*\Psi = 0$:

$$\frac{Jz}{U} = \frac{\frac{\mu}{U} - n}{\lambda(n+1)}.$$



- Both graphs for $\frac{Jz}{U} = 0.08$
- Orange: Rayleigh-Schrödinger mean-field [9]

Numeric Order Parameter

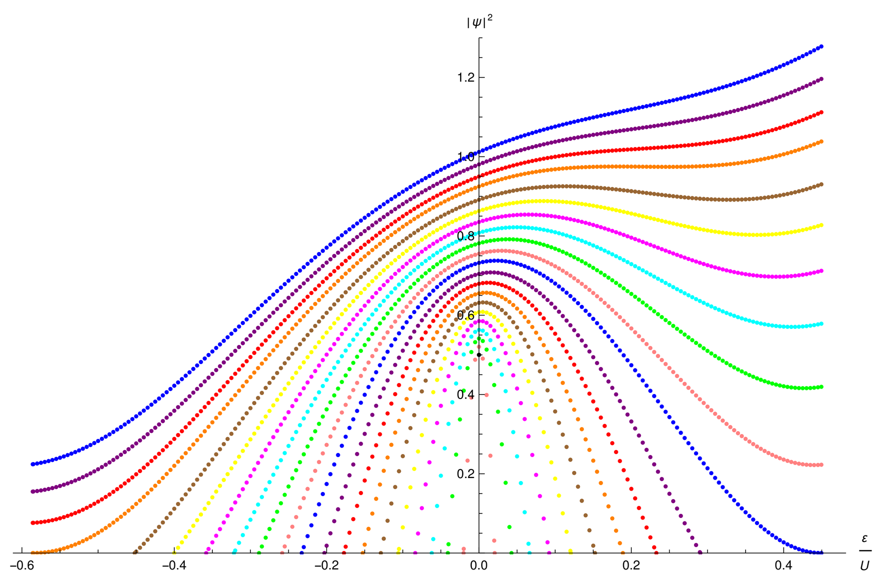
- E_n and $\Psi^*\Psi$ determined by two equations up to quadratic order in λ:

$$\text{Det}\begin{pmatrix} \mathcal{E}_n^{(0)} - E_n + \lambda^2\frac{J^2z^2\Psi^*\Psi n}{E_n - \mathcal{E}_{n-1}^{(0)}} + \lambda^4\frac{J^4z^4\Psi^{*2}\Psi^2 n(n-1)}{\left(E_n - \mathcal{E}_{n-1}^{(0)}\right)^2\left(E_n - \mathcal{E}_{n-2}^{(0)}\right)} & \lambda Jz\Psi^*\sqrt{n+1} \\ \lambda Jz\Psi\sqrt{n+1} & \mathcal{E}_{n+1}^{(0)} - E_n + \lambda^2\frac{J^2z^2\Psi^*\Psi(n+2)}{E_n - \mathcal{E}_{n+2}^{(0)}} + \lambda^4\frac{J^4z^4\Psi^{*2}\Psi^2(n+2)(n+3)}{\left(E_n - \mathcal{E}_{n+2}^{(0)}\right)^2\left(E_n - \mathcal{E}_{n+3}^{(0)}\right)} \end{pmatrix} = 0,$$

and applying $\frac{\partial}{\partial\Psi^*}$ for second equation
- Order parameter $\Psi^*\Psi$ for $\frac{Jz}{U} = 0, .., 0.20$ with stepwith $\Delta\frac{Jz}{U} = 0.01$ and $n = 1$
- Order parameter data fit function $\Psi^*\Psi \approx \Phi$ as a function of $\varepsilon = \mu - U$:

$$\Phi\left(\frac{\varepsilon}{U}, \frac{Jz}{U}\right) = \left[0.5 + 1.98\frac{Jz}{U} + 4\left(\frac{Jz}{U}\right)^2 - 12.4\left(\frac{Jz}{U}\right)^3 + 34\left(\frac{Jz}{U}\right)^4\right]$$
$$+ \frac{\varepsilon}{U}\left[0.253 + 1.73\frac{Jz}{U} + 11.6\left(\frac{Jz}{U}\right)^2 - 73.1\left(\frac{Jz}{U}\right)^3 + 205\left(\frac{Jz}{U}\right)^4\right]$$
$$+ \left(\frac{\varepsilon}{U}\right)^2\left[1.67 - 1.61\frac{Jz}{U} + 0.079\left(\frac{Jz}{U}\right)^2 - 0.0278\frac{U}{Jz} - 0.125\left(\frac{U}{Jz}\right)^2\right.$$
$$\left. -1.42\times 10^{-8}\left(\frac{U}{Jz}\right)^4\right] + \ldots$$

The coloured parts coincide with eq. (1) [7].



Convergence

		Powers in λ		
		2	4	6
One-State Approach	E_1	-1.0108081	-1.0102528	-1.0090297
	$\Psi^*\Psi$	0.19862639	0.24896610	0.25601384
Two-State Approach	E_1	-1.0100015	-1.0104087	-1.0104088
	$\Psi^*\Psi$	0.56303521	0.54132128	0.54131277
Numeric Fit	$\Psi^*\Psi$		0.54126256	

- Values for unperturbed ground-state energy E_1 and order parameter $\Psi^*\Psi$
- At $\frac{Jz}{U} = 0.02$ and degeneracy $\varepsilon = 0$

Analytic Phase Boundary

- Already second order matrix contains all contributions to mean-field phase boundary:

$$\Gamma^{(2)} = \begin{pmatrix} \mathcal{E}_n^{(0)} - E_n + \lambda^2\frac{J^2z^2\Psi^*\Psi n}{E_n - \mathcal{E}_{n-1}^{(0)}} & \lambda Jz\Psi^*\sqrt{n+1} \\ \lambda Jz\Psi\sqrt{n+1} & \mathcal{E}_{n+1}^{(0)} - E_n + \lambda^2\frac{J^2z^2\Psi^*\Psi(n+2)}{E_n - \mathcal{E}_{n+2}^{(0)}} \end{pmatrix}$$

- Determinant yields:

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

- Applying $\frac{\partial}{\partial\Psi^*}$ and $\Psi^*\Psi = 0$:

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

- Solve with respect to $\frac{Jz}{U}$ for phase boundary:

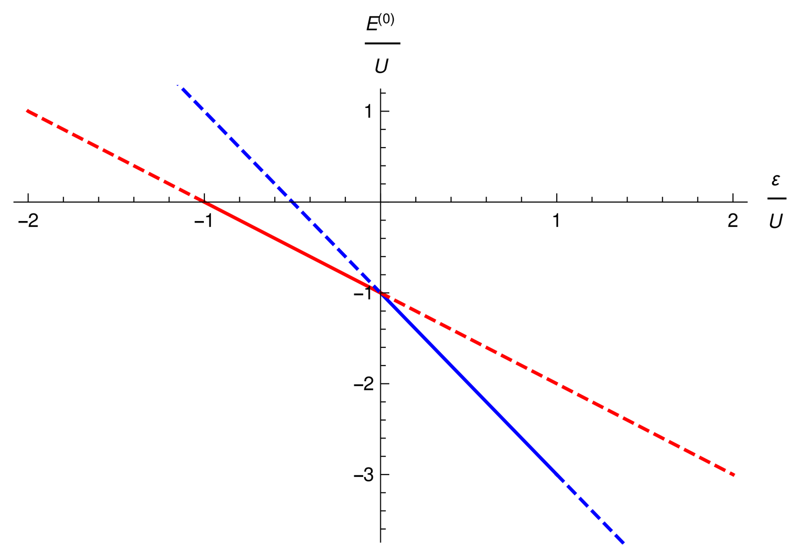
$$\frac{Jz}{U} = \frac{-\left(E_n - E_{n+2}^{(0)}\right)\left(E_n - E_{n-1}^{(0)}\right)\left(2E_n - E_n^{(0)} - E_{n+1}^{(0)}\right)}{U\lambda z\left(3E_n^2(n+1) - E_n\left\{E_{n+2}^{(0)} + 3E_{n-1}^{(0)} + E_n^{(0)}(n+2) + n\left[E_{n+1}^{(0)} + 2\left(E_{n+2}^{(0)} + E_{n-1}^{(0)}\right)\right]\right\} + E_{n-1}^{(0)}\left[E_{n+2}^{(0)} + E_n^{(0)}(n+2) + E_{n+2}^{(0)}n\right] + E_{n+1}^{(0)}E_{n+2}^{(0)}n\right)}$$

- Reduces with Bose Hubbard Hamiltonian and $n = \lambda = 1$:

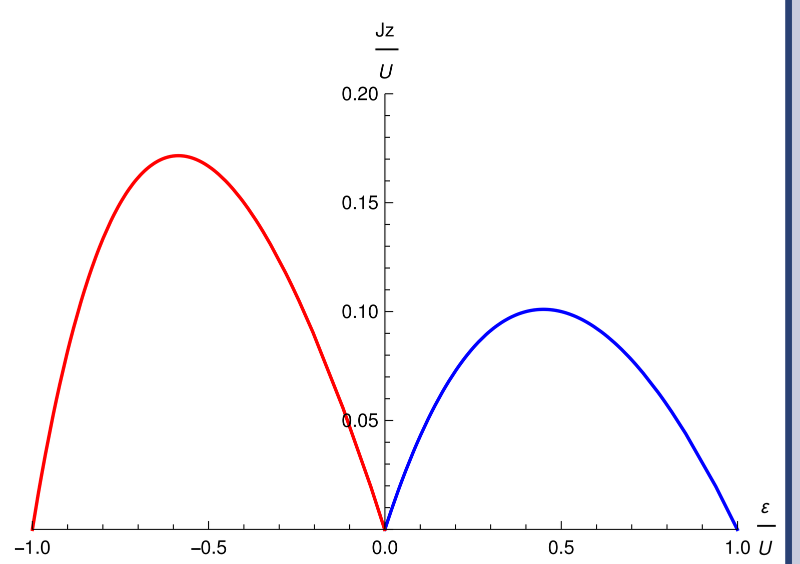
$$\frac{Jz}{U} = -\frac{E_1(3\varepsilon + E_1)(2U + 3\varepsilon + 2E_1)}{3U\varepsilon + 6\varepsilon^2 + 4UE_1 + 14\varepsilon E_1 + 6E_1^2} \qquad (2)$$

- Unperturbed ground-state energy E_1 for $\Psi^*\Psi = 0$:

$$\text{Det}\begin{pmatrix} E_1^{(0)} - E_1 & 0 \\ 0 & E_2^{(0)} - E_1 \end{pmatrix} = 0$$



$E_{n,1} = -1 - \varepsilon$ (red)
$E_{n,2} = -1 - 2\varepsilon$ (blue)



- Insert $E_{n,1}$ in eq. (2) for red lobe
- Insert $E_{n,2}$ in eq. (2) for blue lobe

- Mean-field phase boundary [5] does not change when higher orders in λ are taken into account

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