# B8

# Quantum phase transitions with cold polar molecules

## Quantum corrections for a dipolar BEC in an optical lattice

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## Overview

We study the influence of an external periodic potential on the beyond mean-field corrections in an BEC interacting via contact and dipolar interactions. In a one-dimensional weak lattice, an analytical solution in terms of an effective anisotropic mass is possible to lowest order in the lattice depth. We find isotropic and anisotropic corrections depending on the orientation of the lattice. In the opposite case of a deep optical lattice, we present the lattice Fourier transform of the dipolar interaction potential and show that the energy corrections are enhanced for intermediate ratios of the coherence length of the condensate to the lattice spacing.

### Interacting Bose-Einstein condensate in an external potential $U(\mathbf{r})$

$$H = \int d^3r\, \hat\Psi^\dagger(\mathbf{r}) h_0(\mathbf{r}) \hat\Psi(\mathbf{r}) + \frac{1}{2}\int d^3r\, d^3r'\, \hat\Psi^\dagger(\mathbf{r})\hat\Psi^\dagger(\mathbf{r}') \left(\frac{4\pi\hbar^2 a_s}{m}\delta(\mathbf{r}-\mathbf{r}') + V_{\rm dd}(\mathbf{r}-\mathbf{r}')\right)\hat\Psi(\mathbf{r}')\hat\Psi(\mathbf{r})$$

$$h_0(\mathbf{r}) = -\frac{\hbar^2\nabla^2}{2m} + U(\mathbf{r})$$

contact interaction with s-wave scattering length $a_s$

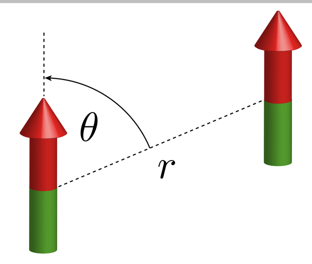
dipolar interaction

### Dipole-dipole interaction

$$V_{\rm dd}(\mathbf{r}) = \frac{C_{\rm dd}}{4\pi}\frac{1-3\cos^2\theta}{r^3}$$

anisotropic

long-range




dipole length $a_{\rm dd} = \frac{C_{\rm dd} m}{12\pi\hbar^2}$

relative strength of dipolar interaction $\varepsilon_{\rm dd} = \frac{a_{\rm dd}}{a_s}$

## Weak lattice

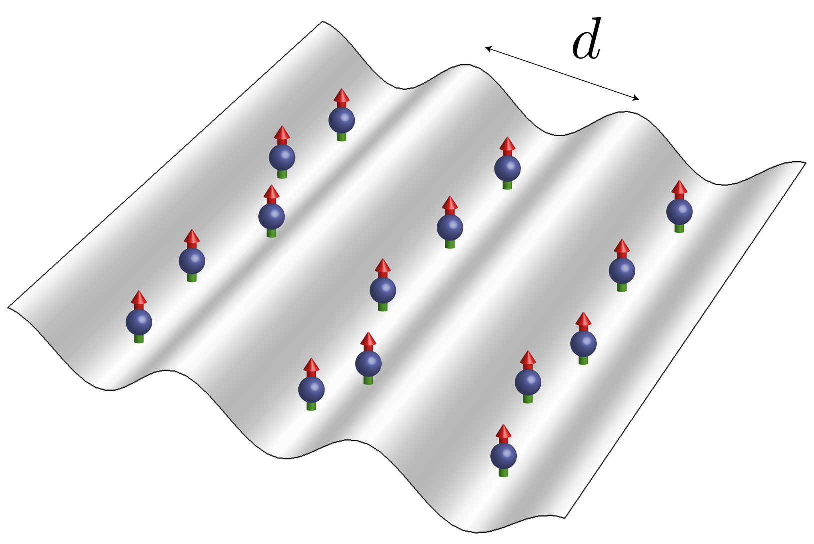
one-dimensional weak lattice

$$U(\mathbf{r}) = U_0 \sin^2(\mathbf{q}\mathbf{r})$$

recoil energy

$$E_R = \frac{\hbar^2|\mathbf{q}|^2}{2m} \qquad |\mathbf{q}| = \frac{\pi}{d}$$

expansion parameter $\quad s = \frac{U_0}{E_R} \ll 1$




determine energy corrections of the ground state in the presence of the lattice consistently to lowest order in $s$

$$\frac{\Delta E_0^s}{V} = \frac{1}{2}\int \frac{d^3k}{(2\pi)^3}\left(E_k^s - E_k^0 - (\varepsilon_k^s - \varepsilon_k^0)\right) \qquad E_k^2 = \varepsilon_k(\varepsilon_k + 2nV_k)$$

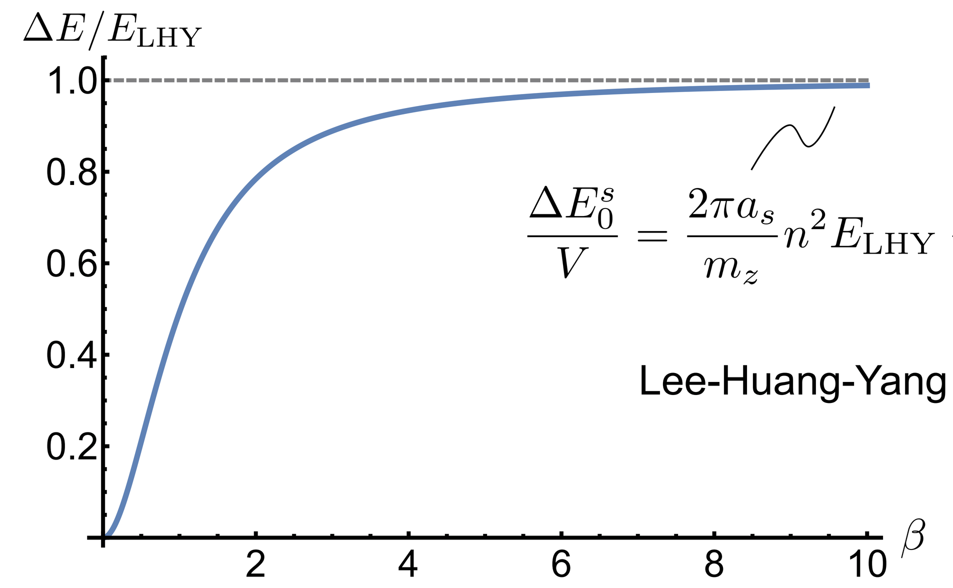
- no corrections to interaction potential to lowest order
- no influence of momenta at the edge of the Brillouin zone in lowest order

### Contact interaction

dimensionless parameter of the problem: $\beta = \pi\frac{\xi}{d}$ $\qquad \xi$ : coherence length

$\beta \to 0$ : influence of the lattice vanishes

$\beta \to \infty$ : problem can be understood in terms of an effective (anisotropic) mass, i.e. $m_z = \left(1 - \frac{s^2}{32}\right) m$




$$\frac{\Delta E_0^s}{V} = \frac{2\pi a_s}{m_z} n^2 E_{\rm LHY} \to \frac{s^2}{64}\frac{2\pi a_s}{m} n^2 E_{\rm LHY} + \mathcal{O}(s^3)$$

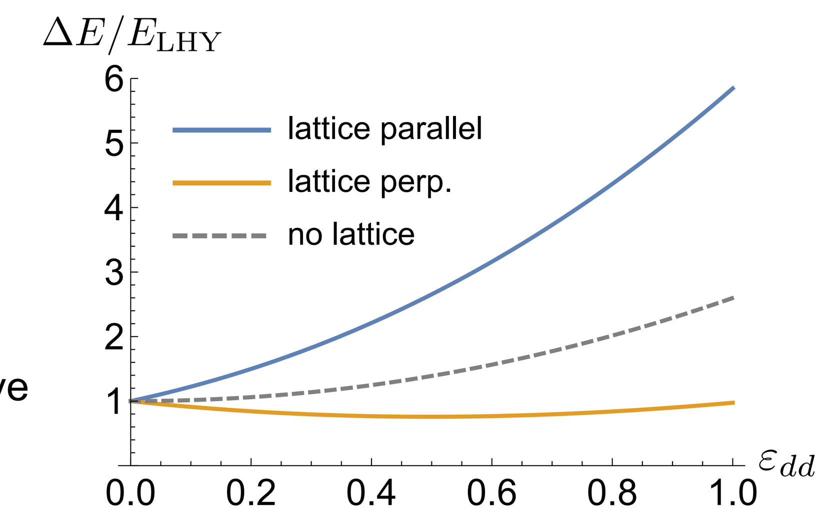
Lee-Huang-Yang correction $\quad E_{\rm LHY} = \frac{128}{15\sqrt{\pi}}\sqrt{na_s^3}$

### Dipole-dipole interaction

calculate energy corrections for $\beta \to \infty$ with anisotropic effective mass

combination of two effects in lowest order:

- isotropic corrections due to presence of the lattice
- anisotropic corrections due to relative orientation of dipoles and lattice




$$\frac{\Delta E_{0,\rm dd}^s}{V} = \frac{s^2}{64}\frac{2\pi a_s}{m} n^2 E_{\rm LHY}\left(F(\varepsilon_{dd}) + \frac{15}{2}\begin{pmatrix}2\\-1\end{pmatrix} G(\varepsilon_{dd})\right)$$

$$F(\varepsilon_{dd}) = \frac{1}{2}\int_{-1}^{1} du\,(1+\varepsilon_{dd}(3u^2-1))^{5/2} \qquad G(\varepsilon_{dd}) = \frac{1}{2}\varepsilon_{dd}\int_{-1}^{1} du\, u^2(1-u^2)(1+\varepsilon_{dd}(3u^2-1))^{3/2}$$

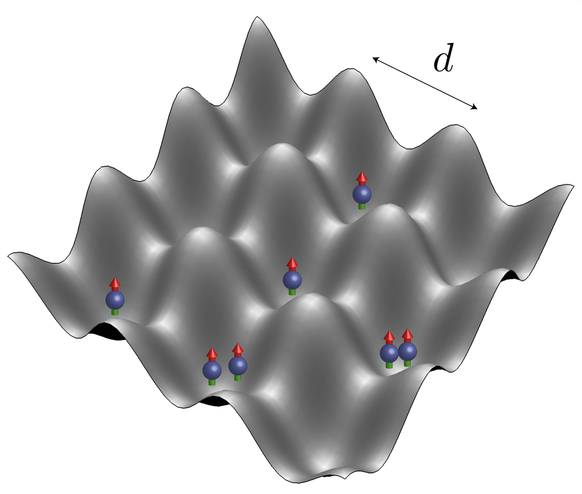
## Deep lattice

3D deep lattice $s \gg 1$, but still in the superfluid regime

- localized wave functions (Wannier functions)

  $\to \quad \hat\psi(\mathbf{r}) = \sum_i w(\mathbf{r}-\mathbf{r}_i)\hat a_i$

- dispersion relation $\quad \varepsilon_k = -2t \sum_{i=x,y,z} \cos(k_i d)$
- momenta are restricted to first Brillouin zone




$t$ : hopping amplitude

### Lattice Fourier transformation of interaction potential

$\delta$-function approximation (width of localized wavefunction $\ll$ lattice spacing)

$$w(\mathbf{r}-\mathbf{r}_i) = \delta(\mathbf{r}-\mathbf{r}_i)$$

$$\to \quad H = \sum_{\mathbf{k}\in K}\varepsilon_k\, \hat a_k^\dagger \hat a_k + \frac{1}{2}\sum_{i,j} V_{ij}\hat a_i^\dagger \hat a_j^\dagger \hat a_j \hat a_i$$

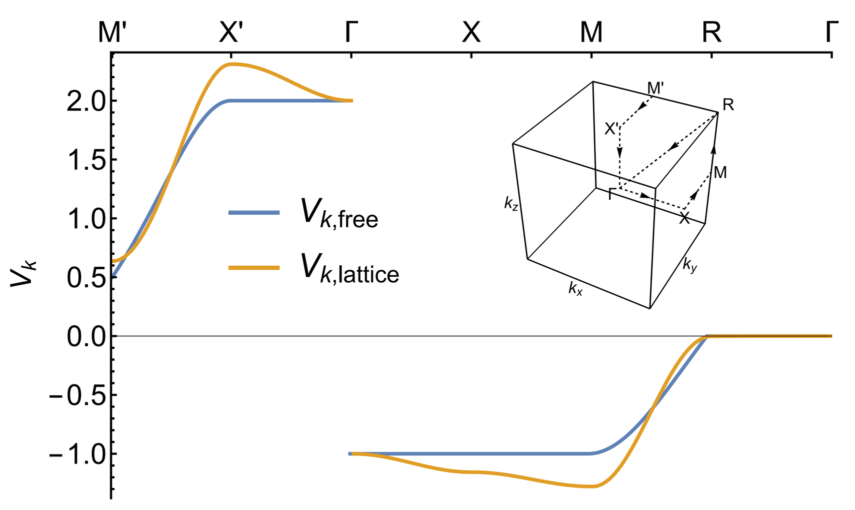
$$V_{ij} = \frac{4\pi\hbar^2 a_s}{m}\left(\delta_{ij} + \varepsilon_{dd}\frac{3}{4\pi}\frac{1-3\cos^2\theta_{ij}}{d^3|i-j|^3}\right)$$

lattice Fourier transformation of dipolar potential

$$V_{\rm dd}(\mathbf{k}) = 3e^{-\frac{k_z^2}{4\pi}}\frac{k_z^2}{k^2} - 1 + \frac{3}{2}\sum_{\mathbf{R}\neq 0}\Big\{\left(E_{-1/2}(\pi R^2) - 2\pi z^2 E_{-3/2}(\pi R^2)\right)e^{i\mathbf{k}\mathbf{R}}$$

$$+2\pi\left(\frac{k_z}{2\pi} + z\right)E_0\left(\pi\left|\mathbf{R} + \frac{\mathbf{k}}{2\pi}\right|^2\right)\Big\} \quad \xrightarrow{\mathbf{k}\to 0} \quad 3\frac{k_z^2}{k^2} - 1$$

$$E_n(x) = \int_1^\infty dt\, \frac{e^{-xt}}{t^n}$$




- displays same non-analytic behaviour at $\mathbf{k} = 0$ as the free space Fourier transform
- corrections to Fourier transform in free space at finite momenta

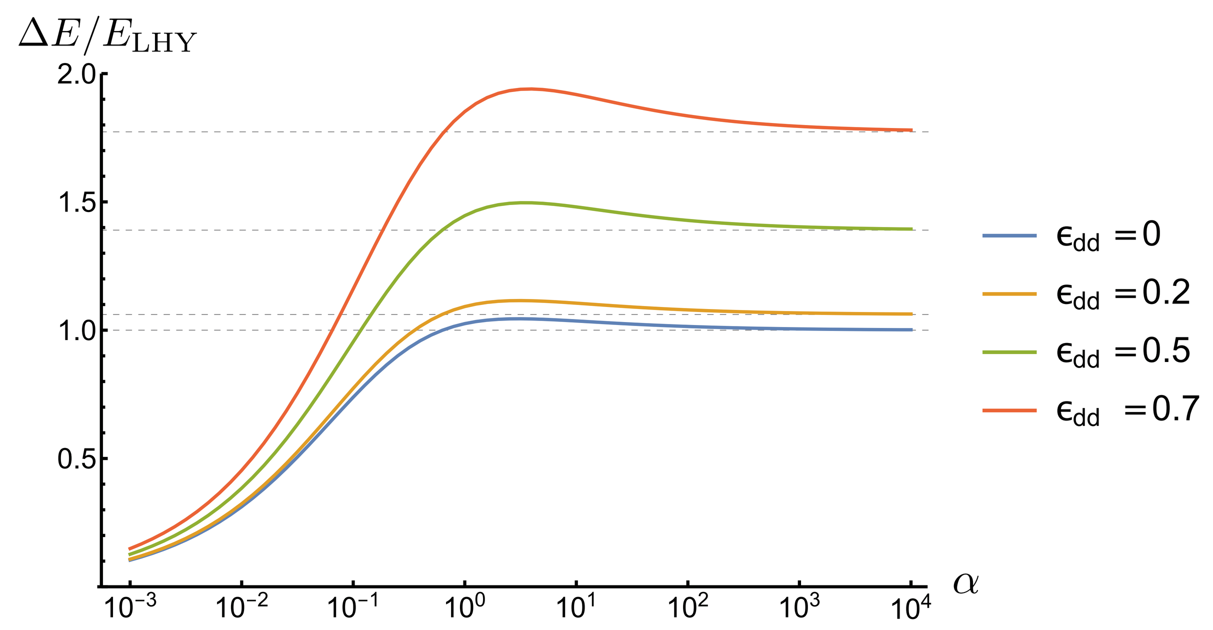
### Energy correction

energy correction depends on dimensionless parameter $\quad \alpha = \frac{\xi^2}{d^2} \sim \frac{t}{na_s}$

$\alpha \to \infty$ : LHY corrections with effective mass $m_{\rm eff} = \frac{\hbar^2}{t\, d^2}$

$$\frac{\Delta E_0}{V} = \frac{2\pi a_s n^2}{m_{\rm eff}}\frac{128}{15\sqrt{\pi}}\sqrt{na_s^3}\, F(\varepsilon_{dd})$$

$\alpha$ finite: energy corrections are enhanced but vanish for small $\alpha$




## Conclusion

**Weak lattice:**

- influence of a weak 1D periodic potential on the beyond mean-field corrections to lowest order in lattice depth
- analytical limit for $d \to 0$ : description using an effective (anisotropic) mass
- isotropic and anisotropic corrections in the case of dipolar interactions

**Deep lattice:**

- beyond mean-field corrections in a strong 3D optical lattice
- calculation of lattice Fourier transform of dipolar potential
  $\to$ corrections to free space result for finite momenta
- enhancement of beyond mean-field corrections for intermediate $\xi/d$

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