Mathematical models for Bose-Einstein condensates in optical lattices (after A. Aftalion and B. Helffer)

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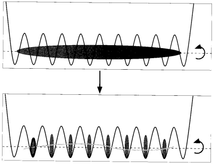
We want to justify the use of some reduced models.
For that purpose, we will use the semi-classical analysis developed for linear problems related to the Schrödinger operator with periodic potential or multiple wells potentials.
In some asymptotic regimes, we justify the reduction to low dimensional problems and in a second step start their study.

[Physical Motivation]

There is a large body of research, both experimental, theoretical and mathematical on vortices in Bose-Einstein condensates [PeSm, PiSt, Af, LSSY].

Current physical interest is in the investigation of very small atomic assemblies, for which one would have one vortex per particle, which is a challenge in terms of detection and signal analysis. An appealing option consists in parallelizing the study, by producing simultaneously a large number of micro-BECs rotating at the various nodes of an optical lattice [Sn]. Experiments are under way.

Our aim, in this paper, is to address mathematical models that describe a BEC in an optical lattice.
The theory is inspired by a series of physics papers [Sn, SnSt, KMPS, STKB].



We want to justify their reduction to simpler energy functionals in certain regimes of parameters and in particular understand the ground state energy.

The ground state energy of a rotating BEC is given by the minimization of

$$Q_{BE,\Omega}(\Psi) := \int_{\mathbb{R}^3} \left(\frac{1}{2} |\nabla \Psi - i\Omega \times \mathbf{r}\Psi|^2 - \frac{1}{2}\Omega^2 r^2 \, |\Psi|^2 + (V(\mathbf{r}) + W_\epsilon(z))|\Psi|^2 + g|\Psi|^4 \right) \, dxdydz \,, \tag{1}$$

under the constraint

$$\int_{\mathbb{R}^3} |\Psi(x,y,z)|^2 \, dxdydz = 1 \,, \tag{2}$$

where

- $r^2 = x^2 + y^2$, $\mathbf{r} = (x,y,z)$,
- Ω is the rotational velocity along the z axis. For simplicity,

$$\Omega \geq 0 \,. \tag{3}$$

- g is the scattering length.

A condensate is a trapped object and the potential $V(\mathbf{r})$ given by

$$V(\mathbf{r}) = \frac{1}{2}\left(\omega_\perp^2 r^2 + \omega_z^2 z^2\right), \tag{4}$$

corresponds to the magnetic trap (= quadratic potential).

We assume that the radial trapping frequency is much larger than the axial trapping frequency :

$$0 \leq \omega_z << \omega_\perp . \tag{5}$$

The experimental data are typically

$$\omega_z/\omega_\perp \sim 5\% .$$

The presence of the one dimensional optical lattice in the z direction is modelled by

$$W_\epsilon(z) = \frac{1}{\epsilon^2} w(z)\,, \tag{6}$$

where

- $\frac{1}{\epsilon^2}$ is the lattice depth,
- w is a positive T-periodic function which admits non-degenerate minima at the points kT $(k \in \mathbb{Z})$:

$$w(z+T) = w(z)\ ,\ w(0) = 0\ ,\ w''(0) > 0\ ,\ w(z) > 0 \text{ if } z \notin T\mathbb{Z}\ . \tag{7}$$

An example is

$$w(z) = \sin^2(\frac{2\pi z}{\lambda}) \tag{8}$$

where λ is the wavelength of the laser light.

We will assume that ϵ tends to 0 (this means deep lattice) and that λ is fixed.

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$$\omega_z = 0 \,. \tag{9}$$

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Actually we mainly discuss, instead of a problem in $\mathbb{R}^3$,

- a periodic problem in the z direction, that is in $\mathbb{R}^2_{x,y} \times [-\frac{T}{2}, \frac{T}{2})$,
- or more generally in $\mathbb{R}^2_{x,y} \times [-\frac{NT}{2}, \frac{NT}{2})$ for a fixed integer $N \geq 1$.

So we focus on the minimization of the functional

$$Q_{BE,\Omega}^{per,N}(\Psi) := \int_{\mathbb{R}^2_{x,y}\times]-\frac{NT}{2},\frac{NT}{2}[} \left(\frac{1}{2}|\nabla\Psi - i\Omega\times\mathbf{r}\Psi|^2 - \frac{1}{2}\Omega^2 r^2|\Psi|^2 + (V(\mathbf{r}) + W_\epsilon(z))|\Psi|^2 + g|\Psi|^4\right) dxdydz\,, \quad (10)$$

under the constraint

$$\int_{\mathbb{R}^2_{x,y}\times]-\frac{NT}{2},\frac{NT}{2}[} |\Psi(x,y,z)|^2\, dxdydz = 1\,, \quad (11)$$

with

$$V(x,y,z) = \frac{1}{2}\omega_\perp^2(x^2+y^2)\,, \quad (12)$$

and Ψ satisfying

$$\Psi(x,y,z+NT) = \Psi(x,y,z)\,. \quad (13)$$

This functional has a minimizer in its natural form domain $\mathcal{D}_{BE,\Omega}^{per,N,unit}$ and we call

$$E_{\Omega}^{per,N} = \inf_{\Psi \in \mathcal{D}_{BE,\Omega}^{per,N,unit}} Q_{BE,\Omega}^{per,N}(\Psi)\,, \tag{14}$$

the groundstate energy of $Q_{BE,\Omega}^{per,N}$.

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$$E^{per,N}_{\Omega} = \inf_{\Psi \in \mathcal{D}^{per,N,unit}_{BE,\Omega}} Q^{per,N}_{BE,\Omega}(\Psi)\,, \tag{14}$$

the groundstate energy of $Q^{per,N}_{BE,\Omega}$.

In the case $N = 1$, we write more simply

$$Q^{per}_{BE,\Omega} := Q^{per,(N=1)}_{BE,\Omega}\,,\ E^{per} := E^{per,(N=1)}_{\Omega}\,. \tag{15}$$

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For that purpose, we will describe how, in certain regimes, the semi-classical analysis developed for linear problems related to the Schrödinger operator with periodic potential or multiple wells potentials is relevant: Outassourt [Ou], Helffer-Sjöstrand [He, DiSj] or for an alternative approach [Si].

The linear model which appears naturally is

$$H = H_\perp^\Omega + H_z \ , \tag{16}$$

with

$$H_\perp^\Omega := -\frac{1}{2}\Delta_{x,y} + \frac{1}{2}\omega_\perp^2 r^2 - i\Omega(x\partial_y - y\partial_x) \ , \tag{17}$$

and

$$H_z := -\frac{1}{2}\frac{d^2}{dz^2} + W_\epsilon(z) \ . \tag{18}$$

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In this situation with separate variables, we can split the spectral analysis, the spectrum of H being the closed set

$$\sigma(H) := \sigma(H_\perp^\Omega) + \sigma(H_z) \,. \tag{19}$$

The first operator $H_\perp^\Omega$ is an harmonic oscillator with discrete spectrum. The bottom of its spectrum is given by

$$\lambda_1^\perp := \inf(\sigma(H_\perp^\Omega)) = \omega_\perp \, . \tag{20}$$

A corresponding groundstate is a Gaussian

$$\psi_\perp = \left(\frac{\omega_\perp}{\pi}\right)^{\frac{1}{2}} \exp -\frac{\omega_\perp}{2} r^2 \, .$$

The gap between the ground state energy and the second eigenvalue (which has multiplicity 1 or 2) is given by

$$\delta_\perp := \lambda_{2,\Omega}^\perp - \lambda_1^\perp = \omega_\perp - \Omega \, . \tag{21}$$

The properties of the periodic Hamiltonian H_z depend on the value of N.

In the case $N = 1$, we call the groundstate $\phi_1(z)$ and the ground energy λ_1^z. In the semi-classical regime $\epsilon \to 0$, λ_1^z satisfies

$$\lambda_1^z \sim \frac{c}{\epsilon}, \tag{22}$$

for some $c > 0$.

The splitting δ_z between the groundstate energy and the first excited eigenvalue satisfies

$$\delta_z \sim \frac{\tilde{c}}{\epsilon}\,, \tag{23}$$

for some $\tilde{c} > 0$.

For $N > 1$, the groundstate energy is unchanged and the corresponding groundstate ϕ_1^N is the periodic extension of ϕ_1 considered as an (NT)-periodic function.
The precise relation is

$$\phi_1^N = \frac{1}{\sqrt{N}}\phi_1 \ , \tag{24}$$

on the line.
But we have now N exponentially close to λ_1^z lying in the first band of the spectrum of the spectral problem for H_z on the whole line. They are separated from the $(N+1)$-th by δ_z^N, with :

$$\delta_z^N = \delta_z + \widetilde{\mathcal{O}}(\exp -S/\epsilon)) \ . \tag{25}$$

Here $\widetilde{\mathcal{O}}(\exp -S/\epsilon))$ means $\mathcal{O}(\exp -\frac{S'}{\epsilon})$, $\forall S' < S$.

The corresponding eigenfunctions satisfy

$$\phi_\ell^N(z+T) = \exp(\frac{2i\pi(\ell-1)}{N})\phi_\ell^N(z)\,, \quad \text{for } \ell = 1,\dots,N\,, \qquad (26)$$

corresponding to the special values $k = \frac{2\pi(\ell-1)}{NT}$ of is usually called a k-Floquet condition.

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We will sometimes use another orthonormal basis (called (NT)-periodic Wannier functions basis) (ψ_j^N) ($j = 0,\dots,N-1$) of the spectral space attached to the N first eigenvalues.

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Each of these (NT)-periodic functions have the advantage to be localized (as $\epsilon \to 0$) in a specific well of W_ϵ considered as defined on $\mathbb{R}/(NT)\mathbb{Z}$.

Using the spectral analysis of the linear problem, there are two natural ideas to compute upper bounds :

- either use test functions of the type

$$\Psi(x,y,z) = \phi(z)\psi_\perp(x,y)\ , \tag{27}$$

where $\psi_\perp$ is the first normalized eigenfunction of $H_\perp^\Omega$ and minimize among all possible L^2-normalized $\phi(z)$ to obtain a $1D$-longitudinal reduced problem,

- or use
  - in the case $N = 1$,

$$\Psi(x, y, z) = \phi_1(z)\psi(x, y) \tag{28}$$

    where ϕ_1 is the first eigenfunction of H_z and minimize among all possible L^2-normalized $\psi(x, y)$ to obtain a $2D$-transverse reduced problem,
  - or in the case $N > 1$

$$\Psi(x, y, z) = \sum_{j=0}^{N-1} \psi_j^N(z)\psi_{j,\perp}(x, y) \tag{29}$$

    where $\psi_j^N(z)$ is the orthonormal basis of Wannier functions mentioned above, and minimize on the suitably normalized $\psi_{j,\perp}$'s which provide N coupled problems.

Computing the energy of a test function of type (27), we get

$$Q_{BE,\Omega}^{per,N}(\Psi) = \omega_\perp + \mathcal{E}_A^N(\phi) \tag{30}$$

where $\mathcal{E}_A^N$ is the functional on the NT-periodic functions in the z direction, defined on $H^1(\mathbb{R}/NT\mathbb{Z})$ by

$$\phi \mapsto \mathcal{E}_A^N(\phi) = \int_{-\frac{NT}{2}}^{\frac{NT}{2}} \left(\frac{1}{2}|\phi'(z)|^2 + W_\epsilon(z)|\phi(z)|^2 + \widehat{g}\,|\phi(z)|^4\right) \, dz \tag{31}$$

with

$$\widehat{g} := g\left(\int_{\mathbb{R}^2} |\psi_\perp(x,y)|^4 \, dxdy\right) = \frac{1}{2\pi} g\omega_\perp . \tag{32}$$

The functional $\mathcal{E}_A^N$ was for example considered in [KMPS].

For test functions of type (28), we get in the case $N = 1$

$$Q^{per}_{BE,\Omega}(\Psi) = \lambda_1^z + \mathcal{E}_{B,\Omega}(\psi) \tag{33}$$

with

$$\mathcal{E}_{B,\Omega}(\psi) := \int_{\mathbb{R}^2_{x,y}} \left(\frac{1}{2}|\nabla_{x,y}\psi - i\Omega \times \mathbf{r}\psi|^2 - \frac{1}{2}\Omega^2 r^2 |\psi|^2 + \frac{1}{2}\omega_\perp^2 (x^2+y^2)|\psi|^2 + \widetilde{g}|\psi|^4 \right) dx\, dy\ , \tag{34}$$

and

$$\widetilde{g} := g \left(\int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4\, dz \right)\ . \tag{35}$$

In the case $N > 1$, we define $\mathcal{E}^N_{B,\Omega}((\psi_{j,\perp})_{j=0,\dots,N-1})$ by

$$Q^{per,N}_{BE,\Omega}(\Psi) = \lambda^z_1 \sum_j ||\psi_{j,\perp}||^2 + \mathcal{E}^N_{B,\Omega}((\psi_{j,\perp})) \tag{36}$$

with

$$\Psi = \sum_{j=0}^{N-1} \psi^N_j(z)\psi_{j,\perp}(x,y)\,.$$

Of course when minimizing over normalized Ψ's, one gets more simply

$$Q_{BE,\Omega}^{per,N}(\Psi) = \lambda_1^z + \mathcal{E}_{B,\Omega}^N((\psi_{j,\perp}))\ .$$

This reduction (or more precisely a simplified approximation of this functional) is proposed in [Sn] on the basis of formal computations. The functional $\mathcal{E}_{B,\Omega}^N$ is somehow related to the Lawrence-Doniach model for superconductors (see [ABB1, ABB2]).

The analysis of the linear case leads immediately to the following trivial and universal inequalities (which are valid for any N and any Ω such that $|\Omega| < \omega_\perp$)

$$\lambda_1^z + \omega_\perp \leq E_\Omega^{per,N} \leq \lambda_1^z + \omega_\perp + I_N \tag{37}$$

where

$$I_N := \frac{g\omega_\perp}{2N\pi} \left(\int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4 dz \right) = \frac{I}{N} \,. \tag{38}$$

This universal estimate is obtained by considering as test function

$$\Psi^{per,N}(x,y,z) = \psi_\perp(x,y)\phi_1^N(z) \,,$$

where ϕ_1^N is the N-th normalized ground state introduces in (24) and $\psi_\perp(x,y)$ is the ground state of $H_\perp^\Omega$, actually independent of Ω.

A rather easy semi-classical analysis shows that $\lambda_1^z + \omega_\perp$ is a good asymptotic of $E_\Omega^{per,N}$ in the limit $\epsilon \rightarrow 0$ when g is sufficiently small (what we can call the quasi-linear situation). More precisely, we have

Theorem QL

Under the condition that either

$$(QLa) \quad g << \epsilon^{\frac{1}{2}} \,, \tag{39}$$

or

$$(QLb) \quad g\omega_{\perp}^{\frac{1}{2}} << 1 \,, \tag{40}$$

then we have

$$E_{\Omega}^{per,N} = (\lambda_1^z + \omega_{\perp})\,(1 + o(1)) \,, \tag{41}$$

as $\epsilon \rightarrow 0$.

Each of these conditions implies that I is small relatively to λ_z or to $\omega_{\perp}$.

So our goal is to analyze more interesting cases when no one of these two conditions is satisfied. We justify the reductions to the lower dimensional functionals

- when m_A^N is much smaller than $\delta_\perp$, where
$$m_A^N = \inf_{||\phi||=1} \mathcal{E}_A^N(\phi) \tag{42}$$
(Case A)
- when $m_{B,\Omega}^N$ is much smaller than $1/\epsilon$, the gap between the two first bands, where
$$m_{B,\Omega}^N = \inf_{\sum_j ||\psi_{j,\perp}||^2=1} \mathcal{E}_{B,\Omega}^N((\psi_{j,\perp}))\,. \tag{43}$$
(Case B)

An independent difficulty is then to have more accurate estimates m_A^N and $m_{B,\Omega}^N$ according to the regime of parameters.

We do not have universal estimates for this but have to separate two cases:

- the weak interaction case, where the interaction term (L^4 term) is at most of the same order as the ground state of the linear problem in the same direction
- the Thomas Fermi case where the kinetic energy term is much smaller than the potential and interaction terms.

In what follows, when N is not mentioned in m_A^N, $m_{B,\Omega}^N$, $\mathcal{E}_A^N$, $\mathcal{E}_{B,\Omega}^N$, then the notations are for $N = 1$. Similarly, if Ω is not mentioned, this means that either the considered quantity is independent of Ω or that we are treating the case $\Omega = 0$. To mention the dependence on other parameters, we will sometimes explicitly write this dependence like for example $m_A^N(\epsilon, \hat{g})$ or $m_{B,\Omega}^N(\epsilon, g, \omega_\perp)$.

We consider states which are of type (27) with $\varphi \in L^2(\mathbb{R}_z/(NT)\mathbb{Z})$. The energy of such test functions provides the upper bound

$$E_{\Omega}^{per,N} \leq \omega_{\perp} + m_A^N(\epsilon, \widehat{g}) \qquad (44)$$

where m_A^N is given by (42).
In order to estimate m_A^N, we first address the "Weak Interaction" case where

$$(AWIa) \quad \frac{1}{\epsilon} << (\omega_{\perp} - \Omega) \, . \qquad (45)$$

and, for a given $c > 0$,

$$(AWIb) \quad g\omega_{\perp}\sqrt{\epsilon} \leq c \, . \qquad (46)$$

Assumption (45) implies that the lowest eigenvalue of the linear problem in the z direction ($\lambda_1^z \sim 1/\epsilon$) is much smaller than the gap in the transverse direction $\delta_\perp = \omega_\perp - \Omega$. This will allow the projection onto the subspace $\psi_\perp \otimes L^2(\mathbb{R}_z/(NT)\mathbb{Z})$.

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Assumption (46) implies that the nonlinear term (of order $g\omega_\perp/\sqrt{\epsilon}$) is of the same order as λ_1^z. It implies using (22) that

$$m_A^N \approx \frac{1}{\epsilon}\,. \tag{47}$$

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All these estimates are obtained by rather elementary semi-classical methods.

Thus, by (45), m_A^N is much smaller than $\delta_\perp$. We prove

Theorem AWI

When $\epsilon \to 0$, and under Conditions (45) and (46), we have

$$E_\Omega^{per,N} = \omega_\perp + m_A^N(\epsilon, \widehat{g})\,(1 + o(1))\,. \qquad (48)$$

We now describe the "Thomas-Fermi" regime. We assume

$$(ATFa) \quad g\omega_\perp\sqrt{\epsilon} >> 1\,. \tag{49}$$

$$(ATFb) \quad g\omega_\perp\epsilon^2 << 1\,. \tag{50}$$

$$(ATFc) \quad g^{\frac{5}{12}}\epsilon^{-\frac{1}{6}}\omega_\perp^{\frac{5}{12}} << (\omega_\perp - \Omega)^{\frac{3}{8}}\,. \tag{51}$$

Assumption (49) implies that the nonlinear term is much bigger than δ_z. Together with (50), it permits also to estimate m_A^N :

$$m_A^N \leq C\left(\frac{\widehat{g}}{\epsilon}\right)^{\frac{2}{3}}\,. \tag{52}$$

Theorem ATF

When ϵ tends to 0, and under Conditions (49), (50) and (51), we have, as $\epsilon \rightarrow 0$,

$$E_{\Omega}^{per,N} = \omega_{\perp} + m_A^N(\epsilon, \widehat{g})\,(1 + o(1))\,. \tag{53}$$

The proofs give actually a much stronger result.

This corresponds to the idea of a reduction on the ground eigenspace in the z variable, where the interaction term is kept in the transverse problem. We recall that we denote by λ_1^z the ground state energy of H_z^{per} and by ϕ_1^N the normalized ground state. We consider states which are of type (28), that is in $L^2(\mathbb{R}^2_{x,y}) \otimes \phi_1(z)$. The energy of such test functions provides the upper bound

$$E_\Omega^{per,N} \leq \lambda_1^z + m_{B,\Omega}^N(\epsilon, g, \omega_\perp)\,. \tag{54}$$

Note the relevant parameter $\tilde{g}$ satisfies

$$\tilde{g} = \frac{g}{N}\left(\int_{-\frac{T}{2}}^{\frac{T}{2}} \phi_1(z)^4 dz\right) \approx \frac{g}{N\sqrt{\epsilon}}\,. \tag{55}$$

In the Weak Interaction case, we prove the following:

Theorem BWI

When ϵ tends to 0, and under the conditions

$$(BWIa) \quad g\epsilon^{-\frac{1}{2}} \leq C \,, \tag{56}$$

$$(BWIb) \quad \omega_\perp \epsilon << 1 \,, \tag{57}$$

then

$$E_\Omega^{per,N} = \lambda_1^z + m_{B,\Omega}^N(\epsilon, g, \omega_\perp)(1 + o(1)) \,. \tag{58}$$

Condition (BWIb) implies that the bottom of the spectrum of the linear problem in the $x - y$ direction is much smaller than δ_z, the gap in the z direction, which is of order $1/\epsilon$. In this case m_B is of

In the Thomas-Fermi case, we prove

Theorem BTF

When ϵ tends to 0, and under the conditions

$$(BTFa) \quad \sqrt{\epsilon} << g \, , \tag{59}$$

$$(BTFb) \quad \omega_\perp \sqrt{g} \epsilon^{\frac{3}{4}} << 1 \, , \tag{60}$$

and

$$(BTFc) \quad g^{\frac{3}{2}} \epsilon^{\frac{1}{4}} \omega_\perp << 1 \, , \tag{61}$$

then

$$E_\Omega^{per,N} = \lambda_1^z + m_B^N(\epsilon, g, \omega_\perp)(1 + o(1)) \, . \tag{62}$$

One can show that, under these assumptions, the term m_B^N is bounded by $\omega_\perp \sqrt{g}/\epsilon^{1/4}$ and thus is much smaller than δ_z which is of order $\frac{1}{\epsilon}$.
Our proofs are made up of two parts: a precise estimate of m_A^N and m_B^N on the one hand, and a lower bound for $E_\Omega^{per,N}$ on the other hand. The lower bound consists in showing that the upperbound obtained by projecting on the special states introduced above in (27), (28) or (29) is actually also asymptotically a good lower bound.

For simplicity, we look at Case A. Recalling that $\delta_\perp = \omega_\perp - \Omega$:

Proposition A

$\exists C > 0$ s. t. $\forall \epsilon \in]0,1]$, $\forall \omega_\perp, \Omega$ s.t. $\delta_\perp \geq 1$, $\forall g \geq 0$,

$$\inf_{||\Psi||=1} \mathcal{E}^{per,N}_{BE,\Omega}(\Psi) = \omega_\perp + m^N_A(\epsilon, \widehat{g})\left(1 - C r_A(\epsilon, \widehat{g})\right) \,, \qquad (63)$$

with

$$\begin{aligned} 0 &\leq r_A(\epsilon, \widehat{g}) \\ &\leq g^{1/4} \delta_\perp^{-\frac{1}{8}} \left(\frac{\delta_\perp + \omega_\perp}{\delta_\perp}\right)^{\frac{1}{4}} \; m^N_A(\epsilon, \widehat{g})^{\frac{1}{4}} \\ &\quad + m^N_A(\epsilon, \widehat{g}) {\delta_\perp}^{-1} \,. \end{aligned} \qquad (64)$$

We describe the proof for $N = 1$ and $\Omega = 0$. We call m_A the infimum instead of m_A^N.
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We project a minimizer Ψ onto $\psi_\perp \otimes L^2(\mathbb{R}/T\mathbb{Z})$, and call $\psi_\perp(x, y)\,\xi(z)$ its projection :

$$\Psi(x, y, z) = \psi_\perp(x, y)\xi(z) + w(x, y, z) \tag{65}$$

with

$$\int_{\mathbb{R}^2} \psi_\perp(x, y) w(x, y, z)\, dxdy = 0\,. \tag{66}$$

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with

$$\int_{\mathbb{R}^2} \psi_\perp(x,y) w(x,y,z)\, dxdy = 0\,. \qquad (66)$$

The orthogonality condition implies

$$1 = \int_{-\frac{T}{2}}^{\frac{T}{2}} |\xi(z)|^2\, dz \; + \; \int_{\mathbb{R}^2\times]-\frac{T}{2},\frac{T}{2}[} |w(x,y,z)|^2\, dxdydz \qquad (67)$$

Now we have the lower bound

$$\int_{-\frac{T}{2}}^{\frac{T}{2}} \mathcal{E}'_B(w(\cdot,\cdot,z))\, dz \geq (\delta_\perp + \omega_\perp) \int_{\mathbb{R}^2 \times]-\frac{T}{2},\frac{T}{2}[} |w(x,y,z)|^2 \, dxdydz \,, \tag{68}$$

with

$$\mathcal{E}'_B(\psi) = \int_{\mathbb{R}^2} \left(\frac{1}{2} |\nabla_{x,y} \psi(x,y)|^2 + \frac{\omega_\perp^2}{2} (x^2 + y^2) \, |\psi(x,y)|^2 \right) \, dxdy \,.$$

We compute the energy of Ψ and use the orthogonality condition so that

$$\mathcal{E}(\Psi) = \omega_\perp \int_{-\frac{T}{2}}^{\frac{T}{2}} |\xi(z)|^2\, dz + \mathcal{E}'_A(\xi) + \int_{\mathbb{R}^2} \mathcal{E}'_A(w(x,y,\cdot))\, dxdy + \int_{-\frac{T}{2}}^{\frac{T}{2}} \mathcal{E}'_B(w(\cdot,\cdot,z))\, dz + g \int_{\mathbb{R}^2\times]-\frac{T}{2},\frac{T}{2}[} |\Psi(x,y,z)|^4\, dxdydz\,, \quad (69)$$

where

$$\mathcal{E}'_A(\phi) = \int_{-\frac{T}{2}}^{\frac{T}{2}} \left(\frac{1}{2}|\phi'(z)|^2 + W_\epsilon(z)|\phi|^2 \right) dz\,.$$

From (67) and (69), we find

$$\mathcal{E}(\Psi) \geq \omega_\perp + \frac{\delta_\perp}{\delta_\perp + \omega_\perp} \int_{-\frac{T}{2}}^{\frac{T}{2}} \mathcal{E}'_B(w(\cdot,\cdot,z))\, dz + \int_{\mathbb{R}^2} \mathcal{E}'_A(w(x,y,\cdot))\, dxdy\,. \tag{70}$$

We use (70) together with the upper bound (44) and (68) to derive that

$$\int_{\mathbb{R}^2\times]-\frac{T}{2},\frac{T}{2}[} |w(x,y,z)|^2\, dxdydz \leq \frac{m_A(\epsilon,\widehat{g})}{\delta_\perp}\,. \tag{71}$$

Note that the righthand side in (71) is very small according to the conditions of the theorem.
Note that (71) implies

$$\int_{-\frac{T}{2}}^{\frac{T}{2}} |\xi(z)|^2 dz \geq 1 - \frac{m_A(\epsilon, \widehat{g})}{\delta_\perp}\,. \tag{72}$$

Then, we get also,

$$\begin{aligned} &\int_{\mathbb{R}^2\times]-\frac{T}{2},\frac{T}{2}[} |\nabla_{x,y} w(x,y,z)|^2\, dxdydz \leq 2\frac{\delta_\perp+\omega_\perp}{\delta_\perp}\; \frac{m_A(\epsilon,\widehat{g})}{\omega_\perp}, \\ &\int_{\mathbb{R}^2\times]-\frac{T}{2},\frac{T}{2}[} |\partial_z w(x,y,z)|^2\, dxdydz \leq 2\; m_A(\epsilon,\widehat{g})\,. \end{aligned} \tag{73}$$

The Sobolev embedding of $H^1(\mathbb{R}^2 \times]-\frac{T}{2},\frac{T}{2}[)$ in $L^6(\mathbb{R}^2 \times]-\frac{T}{2},\frac{T}{2}[)$ gives

$$\|w\|_6 \leq C \|\partial_x w\|_2^{1/3} \|\partial_y w\|_2^{1/3} \left(\|\partial_z w\|_2^2 + ||w||_2^2\right)^{1/6} , \qquad (74)$$

where $|| \cdot ||_p$ denotes the norm in $L^p(\mathbb{R}^2_{x,y} \times]-\frac{T}{2},\frac{T}{2}[)$.

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where $\|\ \cdot\ \|_p$ denotes the norm in $L^p(\mathbb{R}^2_{x,y}\times]-\frac{T}{2},\frac{T}{2}[)$.
So we obtain :

$$\|w\|_6 \leq \tilde{C}m_A(\epsilon,\widehat{g})^{\frac{1}{2}}\left(\frac{\delta_\perp+\omega_\perp}{\delta_\perp}\right)^{\frac{1}{3}}\,. \tag{75}$$

Since by Hölder's Inequality,

$$\|w\|_4 \leq \|w\|_2^{1/4} \|w\|_6^{3/4} ,$$

we deduce that

$$\|w\|_4 \leq C\, m_A(\epsilon, \widehat{g})^{\frac{1}{2}} \delta_\perp{}^{-\frac{1}{8}} \left(\frac{\delta_\perp + \omega_\perp}{\delta_\perp} \right)^{\frac{1}{4}} . \qquad (76)$$

We expand

$$|\Psi|^4 = |\psi_\perp|^4|\xi|^4 + 2|\psi_\perp|^2|\xi|^2|w|^2 \\ +4(\Re(\psi_\perp\xi\overline{w}) + \frac{1}{2}|w|^2)^2 + 4|\psi_\perp|^2|\xi|^2\Re(\psi_\perp\xi\overline{w}) \,.$$

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Since (69) implies that

$$\mathcal{E}(\Psi) \geq \omega_\perp + \mathcal{E}_A(\xi) - 4g\int_{\mathbb{R}^2\times]-\frac{T}{2},\frac{T}{2}[} |\psi_\perp(x,y)|^3|\xi(z)|^3|w(x,y,z)|\,dxdydz\,,$$

in order to get the lower bound, we just need to prove that the last term is a perturbation to $\mathcal{E}_A(\xi)$.

We can do the following estimates

$$g \int |\psi_\perp(x,y)|^3 |\xi(z)|^3 |w(x,y,z)| \, dxdydz$$
$$\leq c_0 g \omega_\perp^{\frac{3}{4}} \left(\int |\psi_\perp(x,y)|^4 \, dxdy\right)^{\frac{3}{4}} \left(\int |\xi(z)|^4 dz\right)^{\frac{3}{4}} \|w\|_4$$

by Hölder,

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$$\leq c_1 g^{1/4} (\mathcal{E}_A(\xi))^{3/4} \|w\|_4$$

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$$\leq c_0 g \omega_\perp^{\frac{3}{4}} (\int |\psi_\perp(x,y)|^4\, dxdy)^{\frac{3}{4}} \, (\int |\xi(z)|^4 dz)^{\frac{3}{4}} \, \|w\|_4$$

by Hölder,

$$\leq c_1 g^{1/4} (\mathcal{E}_A(\xi))^{3/4} \|w\|_4$$

using the control of the quartic term by the energy,

$$\leq c_2 g^{1/4} {\delta_\perp}^{-\frac{1}{8}} \left(\frac{\delta_\perp + \omega_\perp}{\delta_\perp}\right)^{\frac{1}{4}} \, m_A(\epsilon, \widehat{g})^{\frac{1}{2}} (\mathcal{E}_A(\xi))^{3/4}$$

using the control of $||w||_4$ by the energy,

We can do the following estimates

$$g\int |\psi_\perp(x,y)|^3|\xi(z)|^3|w(x,y,z)|\,dxdydz$$
$$\leq c_0 g\omega_\perp^{\frac{3}{4}}\left(\int |\psi_\perp(x,y)|^4\,dxdy\right)^{\frac{3}{4}}\left(\int |\xi(z)|^4 dz\right)^{\frac{3}{4}}\|w\|_4$$

by Hölder,

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using the control of the quartic term by the energy,

$$\leq c_2 g^{1/4}{\delta_\perp}^{-\frac{1}{8}}\left(\frac{\delta_\perp+\omega_\perp}{\delta_\perp}\right)^{\frac{1}{4}}\; m_A(\epsilon,\widehat{g})^{\frac{1}{2}}(\mathcal{E}_A(\xi))^{3/4}$$

using the control of $||w||_4$ by the energy,

$$\leq c_3\, g^{1/4}{\delta_\perp}^{-\frac{1}{8}}\left(\frac{\delta_\perp+\omega_\perp}{\delta_\perp}\right)^{\frac{1}{4}}\; m_A(\epsilon,\widehat{g})^{\frac{1}{4}}\left(1+C\,m_A(\epsilon,\widehat{g}){\delta_\perp}^{-1}\right)\;\mathcal{E}_A(\xi)\;.$$

Here to get the last line, we have used the lower bound

$$\mathcal{E}_A(\xi)\geq m_A(\epsilon,\widehat{g})\,||\xi||_2^4\,,$$

and (72).

This leads to

$$\mathcal{E}(\Psi) \geq \omega_\perp \\ +\mathcal{E}_A(\xi)\left(1 - C\, g^{1/4}\delta_\perp{}^{-\frac{1}{8}}\left(\frac{\delta_\perp+\omega_\perp}{\delta_\perp}\right)^{\frac{1}{4}} m_A(\epsilon,\widehat{g})^{\frac{1}{4}} - C\, m_A(\epsilon,\widehat{g})\delta_\perp{}^{-1}\right),$$

and then to the proposition.

We just describe the reduced model occuring in the case AWI.

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Using the basis (ψ_j^N) of (NT)-periodic Wannier functions attached to the N first eigenvalues, we consider, as an approximation, the functional

$$\mathbb{C}^N \ni (c)_{j=0,\dots,N-1} \mapsto \mathcal{E}_A^N(\mathbf{c}) = \mathcal{E}_A^N(\sum_{j=0}^{N-1} c_j \psi_j) \,.$$

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Only nearby wells interact by tunneling and semi-classical analysis leads to

$$\lambda_1^z \left(\sum_{j=0}^{N-1} |c_j|^2 \right) - \tau \Re \left(\sum_{j=0}^{N-1} c_j\, \overline{c_{j+1}} \right) + \widehat{g}\,(\sum_{j=0}^{N-1} |c_j|^4)\,(\int_{-\frac{NT}{2}}^{\frac{NT}{2}} |\psi_0^N(z)|^4\, dz) \tag{77}$$

where $\tau \sim c\epsilon^{-3/2} e^{-S/\epsilon}$, and $c_N = c_0$.

So we get the question of analyzing the Discrete Nonlinear Schrödinger model :

$$D(\mathbf{c}) = -\tau \sum_{j=0}^{N-1} (\overline{c_j} c_{j+1} + c_j \overline{c_{j+1}}) + I \sum_{j=0}^{N-1} |c_j|^4 \,,$$

with two parameters I and τ.

This model is considered by Macholm, Nicholin, Pethick, Smith.

After some additional approximations the functional becomes

$$\begin{aligned}\mathcal{E}_B^{N,approx}((\psi_{j,\perp})_j) \quad &= \sum_{j=0}^{N-1} \int_{\mathbb{R}^2} \big(|(\nabla_{x,y} - i\Omega \times \mathbf{r})\psi_{\perp,j}|^2 \\ &\qquad + V(x,y)|\psi_{j,\perp}(x,y)|^2\big)\ dxdy \\ &+ s \sum_{j=0}^{N-1} ||\psi_{j,\perp}||^2 \\ &+ t \sum_{j=0}^{N-1} \left(\langle \psi_{j,\perp}, \psi_{j+1,\perp}\rangle + \langle \psi_{j,\perp}, \psi_{j-1,\perp}\rangle\right) \\ &+ \widetilde{g} \sum_{j=0}^{N-1} ||\psi_{j,\perp}||_{L^4}^4\ ,\end{aligned} \tag{78}$$

with $V(x,y) = \frac{1}{2}(\omega_\perp^2 - \Omega^2)(x^2+y^2)$, which should be minimized over the $(\psi_{j,\perp})_j$ such that

$$\sum_{j=0}^{N-1} ||\psi_{j,\perp}||^2 = 1\ .$$

This is the model described by Snoek [Sn].

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