Liquid-Solid Transition in ^{4}He at T = 0 K; analytical results about the Ground-State Wave Function

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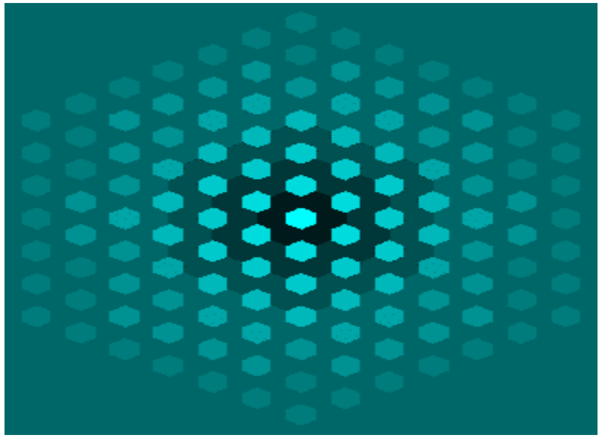
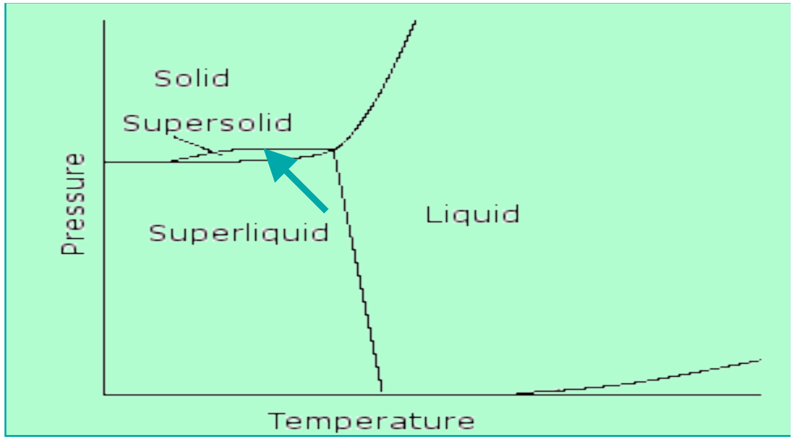


Solid Helium



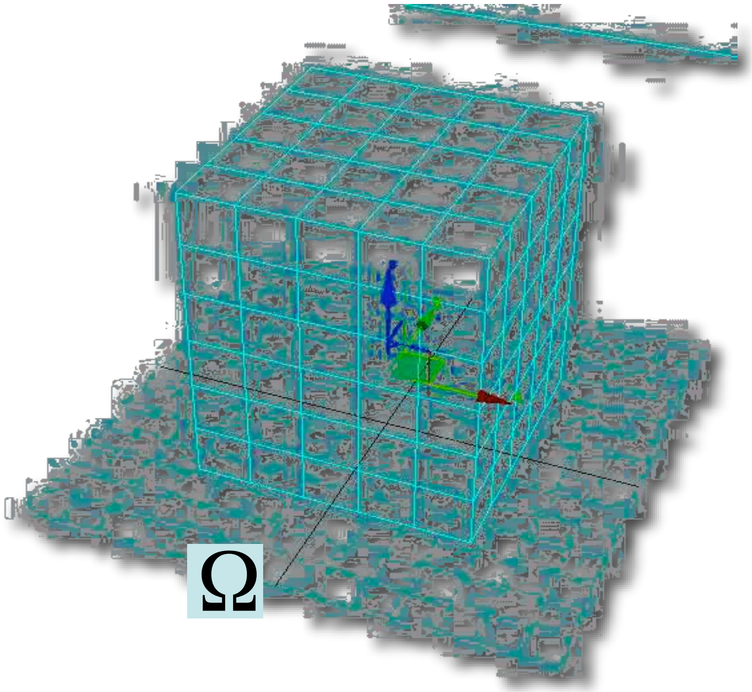
In the crystalline phase, samples of Helium atoms seem to exibit quantum coherence phenomena … "supersolidity"; microscopic models are needed to put light into this new intriguing physical scenario.

At T = 0 K all such methods rely on variational models of the ground state wave function of a "quantum solid".

An open problem regards the transformation properties under translations, whether it would be better to use a wave function translationally invariant, like a *Shadow Wave Function*, (S.A. Vitiello, K.Runge and M.H. Kalos, *Phys. Rev. Lett.* (1988)) in which inter-particles correlations give rise to a mechanism of spontaneously symmetry-breaking, or a wave function which explicitly breaks translational symmetry introducing *a priori* the sites of a crystal lattice, like a *Jastrow-Nosanow Wave Function* (L.H. Nosanow, *Phys. Rev. Lett.* (1964)).

We investigate such symmetry properties of the **exact ground state** of the quantum many body problem.

The model of the system



N spinless structureless bosons confined in a cubic box

$$\Omega \subset R^3$$

To study the bulk properties of the system, we imagine the macroscopic system as a covering of the whole euclidean space made of boxes identical to our confinement region.

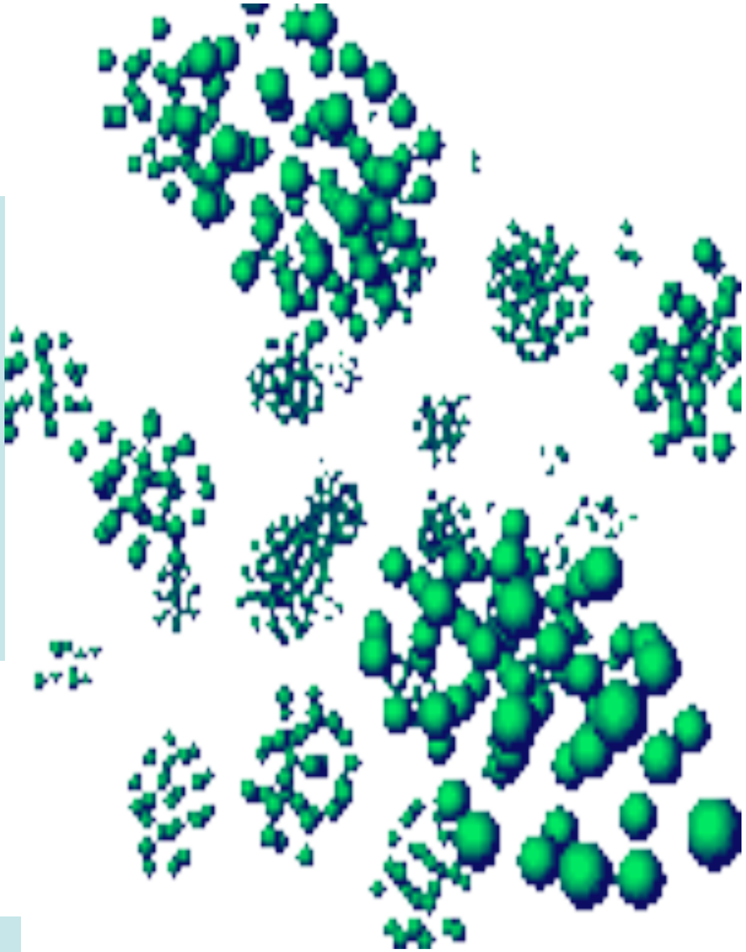
Studying the degrees of freedom in the confinement region, we are making a local description of a macroscopic sample

Mathematical Description

- Hilbert Space of the system:

$$h_{Bose} = \left(\underbrace{L^2(\Omega) \otimes \ldots \otimes L^2(\Omega)}_{N} \right)_{sym}$$

$$h_{Bose} = \left\{ \begin{array}{l} [f] : \int_\Omega dr^N \left| f(\vec{r_1},\ldots,\vec{r_N}) \right|^2 < +\infty, \\ f(\vec{r_1},\ldots,\vec{r_N}) = f(\overrightarrow{r_{\sigma(1)}},\ldots,\overrightarrow{r_{\sigma(N)}}), \forall \sigma \in S_N \end{array} \right\}$$



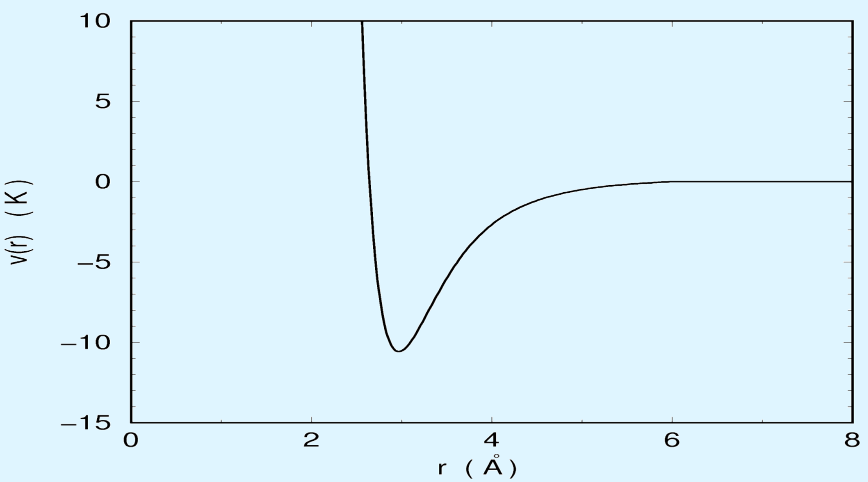
- Hamiltonian Operator

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j=1}^{N} v(\vec{\hat{r}}_i - \vec{\hat{r}}_j)$$

Interaction potential

As a model of effective two-body interaction among ^{4}He atoms we take the Aziz potential (R.A. Aziz, *Mol. Phys., (1987)*)

$$v_{Aziz}(r)=\begin{cases}\varepsilon\left\{Ae^{-\frac{\alpha r}{r_m}}-\left[C_6\left(\frac{r_m}{r}\right)^6+C_8\left(\frac{r_m}{r}\right)^8+C_{10}\left(\frac{r_m}{r}\right)^{10}\right]e^{-\left(\frac{Dr_m}{r}-1\right)^2}\right\}, r\le Dr_m\\ \varepsilon\left\{Ae^{-\frac{\alpha r}{r_m}}-\left[C_6\left(\frac{r_m}{r}\right)^6+C_8\left(\frac{r_m}{r}\right)^8+C_{10}\left(\frac{r_m}{r}\right)^{10}\right]\right\}, r> Dr_m\end{cases}$$



Extension of the interactions to the images

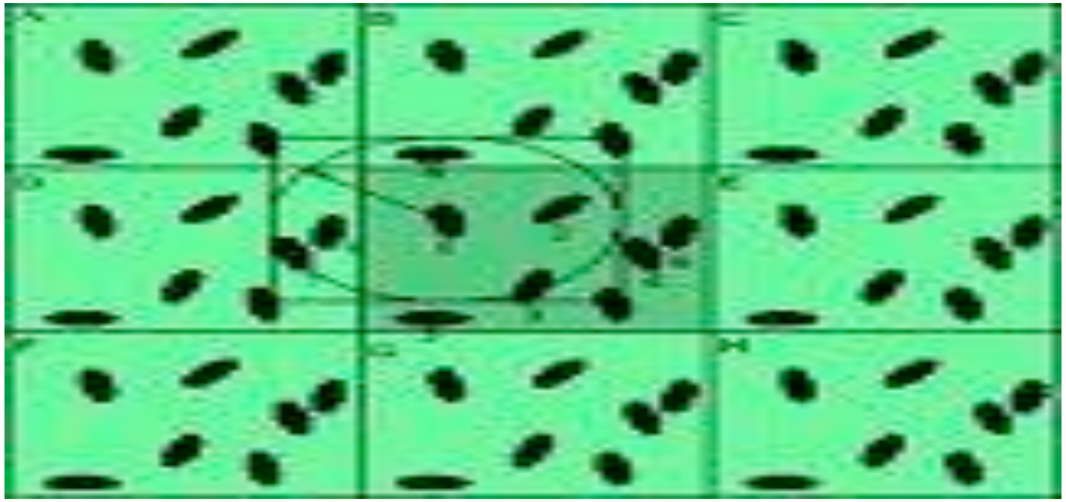
In our picture of the macroscopic system, the N particles in the box interact with the particles in the identical copies of the box; introducing a cutoff distance in the interaction, so that only nearest boxes interact, we write the interaction term in the Hamiltonian

$$\sum_{i<j=1}^{N} v(\vec{r}_i - \vec{r}_j),$$

$$v(\vec{r}_i - \vec{r}_j) \equiv v_{Aziz}\left(\left|\left(\vec{r}_i - \vec{r}_j\right)_{PBC}\right|\right)$$

$$\left(\vec{x}_{PBC}\right)_{\alpha=x,y,z} \equiv x_\alpha - L\,nin\left(\frac{x_\alpha}{L}\right)$$

$$L \equiv \left(V(\Omega)\right)^{1/3}$$



Periodic boundary conditions, domain of the Hamiltonian

$$\hat{H} : D_{\hat{H}} \subset h_{Bose} \longrightarrow h_{Bose}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j=1}^{N} v(\vec{\hat{r}}_i - \vec{\hat{r}}_j)$$

The domain of the Hamiltonian is made of (equivalence classes of) functions in the Hilbert Space of the system, satisfying suitable smoothness properties and **periodic boundary conditions** at the boundaries of the confinement region.

Mathematical results

Since the interaction potential belongs to the "Rollnik class", that is

$$\iint_{\Omega\times\Omega} d^3x d^3y \frac{\left|v(\vec{x})\right|\left|v(\vec{y})\right|}{\left|\vec{x}-\vec{y}\right|^2} < +\infty$$

the hamiltonian operator defines a *compact resolvent* operator densely defined in the Hilbert space of the system, and the "imaginary time evolution operator"

$$e^{-\beta\hat{H}}$$

is *trace-class*

so that one can deduce the following important properties (Reed-Simon, *Methods of modern Mathematical Physics*, vol. II, IV):

Theorem

1) The spectrum of the Hamiltonian coincides with the discrete set of eigenvalues
2) The eigenspaces have finite dimension
3) There exist a s.o.n.c. of eigenfunctions of the Hamiltonian operator, with the sequence of eigenvalues divergent
4) The minimum eigenvalue is non-degenerate and the corresponding eigenfunction is strictly positive

The Ground State wave function

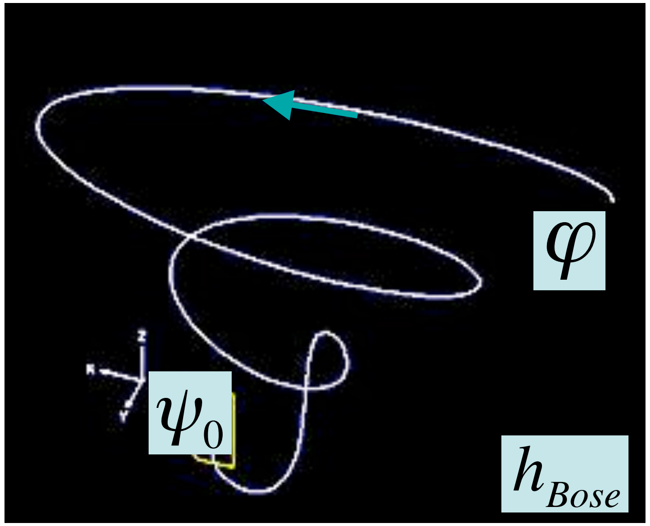
$$\psi_0(\vec{r}_1,\ldots,\vec{r}_N)$$

"Projection" formula:

$$\varphi \in h_{Bose}, \langle \psi_0 | \varphi \rangle \neq 0$$

$$\lim_{\tau \to +\infty} \frac{e^{-\tau(\hat{H}-E_0)}}{\langle \psi_0 | \varphi \rangle} \varphi = \psi_0$$

The limit is taken in the topology of the Hilbert space h_{Bose}



Translational invariance

We are going to prove now the following symmetry property of the Ground State wave function, which holds whenever the number of particles is finite.

$$\psi(\vec{r}_1 - \vec{a}, \ldots, \vec{r}_N - \vec{a}) = \psi_0(\vec{r}_1, \ldots, \vec{r}_N)$$

$$\vec{a} \in R^3$$

If one of the position vectors falls out of the box, we interpret the l.h.s. as the periodic extension of the wave function in the box

Proof

Let us construct a wave function, translationally invariant, with non-zero overlap on the true ground state.

$$\varphi \in h_{Bose}, \varphi(\vec{r}_1 - \vec{a}, \ldots, \vec{r}_N - \vec{a}) = \varphi(\vec{r}_1, \ldots, \vec{r}_N)$$
$$\langle \psi_0 | \varphi \rangle \neq 0$$

Due to the a.e. positivity of the ground state wave function this construction is always possible; for example we may use a ***Jastrow Wave function***

$$\varphi_J(\vec{r}_1, \ldots, \vec{r}_N) = \frac{1}{\sqrt{Q}} \prod_{i<j=1}^{N} e^{-\frac{1}{2}\left(\frac{b}{\left|(\vec{r}_i - \vec{r}_j)_{PBC}\right|}\right)^5}$$

The known result that L^2-convergence implies the existence of a subsequence puntually converging, allows us to write:

$$\psi_0(\vec{r}_1-\vec{a},....,\vec{r}_N-\vec{a})=\frac{1}{\langle\psi_0|\varphi_J\rangle}\lim_{\tau_k\to+\infty}\left(e^{-\tau_k(\hat{H}-E_0)}\varphi_J\right)(\vec{r}_1-\vec{a},....,\vec{r}_N-\vec{a})$$

Since it is simple to show that :

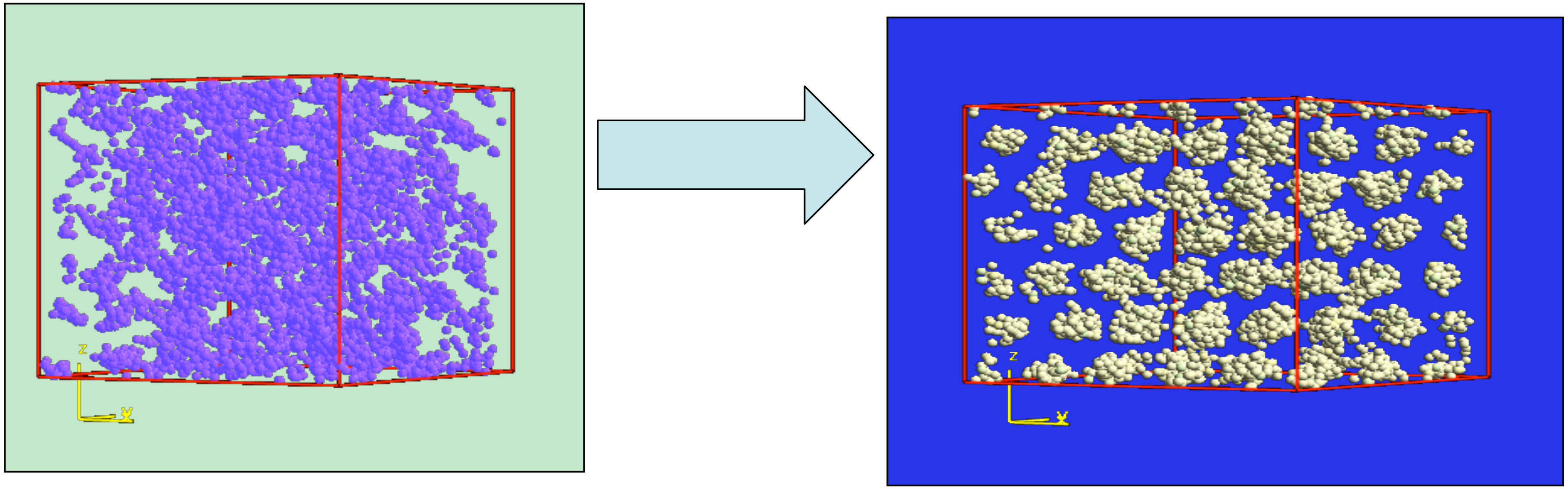
$$\left(e^{-\tau_k(\hat{H}-E_0)}\varphi_J\right)(\vec{r}_1-\vec{a},....,\vec{r}_N-\vec{a})=\left(e^{-\tau_k(\hat{H}-E_0)}\varphi_J\right)(\vec{r}_1,....,\vec{r}_N)$$

we have:

$$\psi_0(\vec{r}_1-\vec{a},....,\vec{r}_N-\vec{a})=\frac{1}{\langle\psi_0|\varphi_J\rangle}\lim_{\tau_k\to+\infty}\left(e^{-\tau_k(\hat{H}-E_0)}\varphi_J\right)(\vec{r}_1-\vec{a},....,\vec{r}_N-\vec{a})=$$
$$=\frac{1}{\langle\psi_0|\varphi_J\rangle}\lim_{\tau_k\to+\infty}\left(e^{-\tau_k(\hat{H}-E_0)}\varphi_J\right)(\vec{r}_1,....,\vec{r}_N)=\psi_0(\vec{r}_1,....,\vec{r}_N)$$

which is the desired result.

Symmetry-breaking



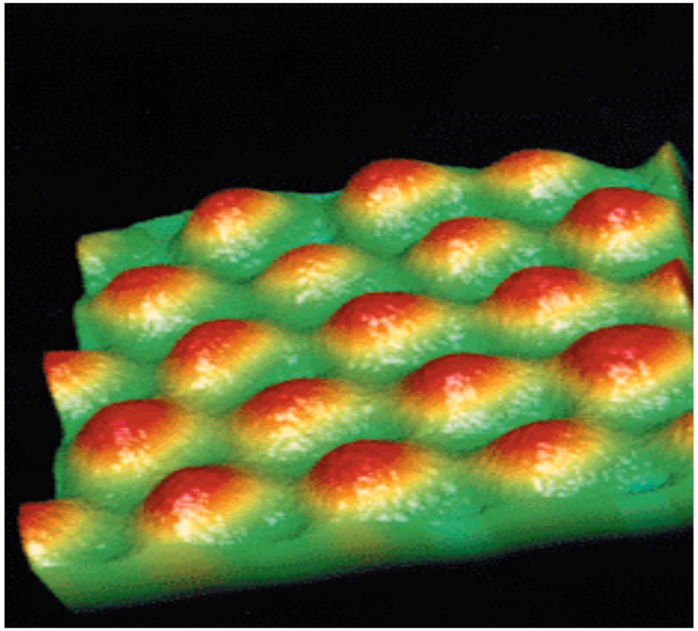
If the average density of Helium atoms, at T = 0 K, exceeds a critical value, the extensive Bragg peaks of the Static Structure factor reveals the presence of a crystalline phase; in a finite system, the crystalline order arises but the center-of-mass motion preserves the translational symmetry, so that the translationally invariant wave function describes the solid phase. In the thermodynamic limit, the super selection rules forbide the center-of-mass motion and the system shows translational symmetry-breaking.

Mathematical model

We have shown that the ground state wave function of the finite system is translationally invariant at any density.
now, we try to induce in the system a periodic modulation in the local density; let's define:

$$\rho_{\vec{q}}(\vec{r}) = \frac{N}{V}\left(1 + \gamma \cos(\vec{q} \cdot \vec{r})\right)$$

$$E_{\vec{q}} = \min_{\left\{\psi \in h_{Bose} : \left\langle \psi \middle| \left(\sum_{i=1}^{N} \delta(\vec{r} - \hat{\vec{r}}_i)\right) \psi \right\rangle = \rho_{\vec{q}}(\vec{r})\right\}} \left\langle \psi \middle| \hat{H} \psi \right\rangle$$



$E_{\vec{q}}$ is the minimum energy in the class of wave functions which give the local density $\rho_{\vec{q}}(\vec{r})$

The Stiffness Theorem

We may evaluate the energy cost of creating such a density modulation using the "Stiffness theorem" about the ground state wave function

$$\delta E_{\vec{q}} \equiv E_{\vec{q}} - E_0 = -\frac{N^2}{4V\chi_{nn}(\vec{q},\omega=0)}\gamma^2$$

where:

$$\chi_{nn}(\vec{q},\omega) = -\frac{i}{\hbar V}\lim_{\eta\to 0^+}\int_0^{+\infty}\left\langle\left[\hat{n}_{\vec{q}}(t),\hat{n}_{-\vec{q}}\right]\right\rangle_0 e^{i(\omega+i\eta)t}dt$$

$\hat{n}_{\vec{q}}$ being the Fourier trasform of the local density operator

A possible mechanism of symmetry-breaking

In the context of linear response theory it is shown that

$$\chi_{nn}(\vec{q},\omega=0)\leq 0$$

So that one could never lower the energy modulating the local density. Despite of that, in the ***thermodynamic limit***, the ground
state can become ***degenerate***, if, for some suitable set of
wave vectors, the static limit of the density-density response function diverges faster than the particles number.

The Bragg Peaks

It has been proved that:

$$\left|\chi_{nn}(\vec{q},\omega=0)\right| \geq \frac{4NmS^2(\vec{q})}{V\hbar^2 q^2}$$

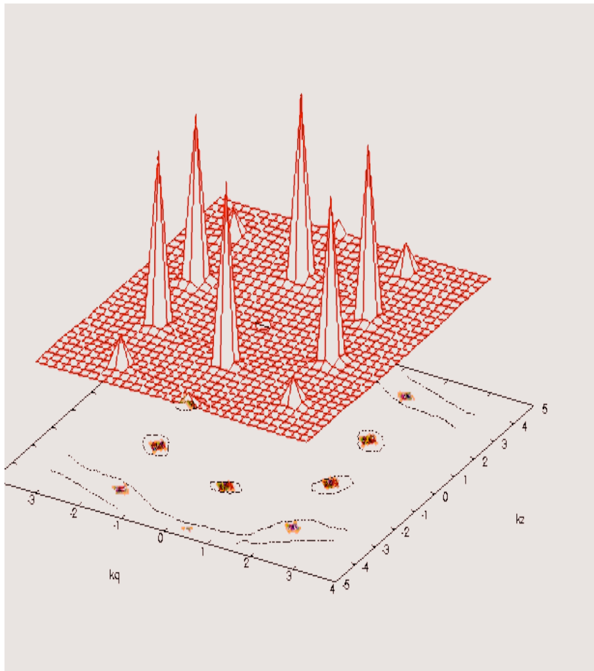
where

$$S(\vec{q}) = \frac{1}{N}\left\langle \hat{n}_{\vec{q}}\hat{n}_{-\vec{q}} \right\rangle_0$$

is the ***Static Structure Factor***

So that we can write:

$$\delta E_{\vec{q}} \leq N \frac{\gamma^2\hbar^2 q^2}{16mS^2(\vec{q})}$$



Local density modulations governed by the set of wave vectors which maximizes the Static Structure Factor, if the average density if high enough so that the Bragg peaks are extensive, cost no energy in the thermodynamic limit.

Conclusions

From this analysis one sees a picture in which inter-particle correlations give rise to a crystalline order in the system, inducing a symmetry breaking mechanism. In our opinion, the explicit introduction of the sites of a crystal lattice in a variational model of the ground state wave function would force the system into a state which could be far from the true equilibrium.

We think advisable to build up variational models translationally invariant, as the true ground state of the finite system, and let the crystalline phase spontaneously arise.