Some Mathematical Questions of Quantum Mechanics

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Schrödinger equation

Many-body quantum systems are described by the Schrödinger eq.

$$i\partial_t \psi = H_n \psi. \tag{SE}$$

where $\psi = \psi(x_1, \ldots, x_n, t)$ and $H_n = n-$particle Schrödinger opr,

$$H_n := \sum_1^n \frac{-1}{2m}\Delta_{x_i} + \sum_{i<j} v(x_i - x_j). \tag{1}$$

(For n particles of mass m interacting via a 2-body potential v.)

Global existence $\Longleftrightarrow$ self-adjointness of H_n

Goal: Describe the space-time behaviour of solutions

Main problem: *stability* vs *decay*.

Stability = localiz. in space & period. in time (atoms, ..., stars):

- *stability w. r. to collapse (lower bounds $H_n \geq -C > -\infty$)*
- *stability w. r. to break-up (gap(*inf H*, rest)* > 0*).*

Decay = Local decay $\Longrightarrow$ Break-up $\Longrightarrow$ scattering

Scattering

The main mathematical problem of the scattering theory - the asymptotic completeness states:

As time progresses, a quantum system settles in a superposition of states in each of which it is broken into a stable freely moving fragments.

Theorem (Asymptotic completeness)

Suppose that the pair potentials $v_{ij}(x_i - x_j)$ entering H_n satisfy $v_{ij}(y) = O(|y|^{-\mu})$, with $\mu > \sqrt{3} - 1$. Then the asymptotic completeness holds.

Open problem: Prove the asymptotic completeness $v_{ij}(y) = O(|y|^{-\mu})$, with $\mu \leq \sqrt{3} - 1$.

Including photons (NR QED)

To describe the real (at least visible) world, have to couple the particles to photons (quantized electromagnetic field) $\Longrightarrow$

$$i\partial_t\psi_t = H_\kappa\psi_t,$$

where H_κ is the hamiltonian on the state space $\mathcal{H} := \mathcal{H}_p \otimes \mathcal{H}_f$:

$$H_\kappa = \sum_{j=1}^{n} \frac{1}{2m}\big(-i\nabla_{x_j} - \kappa A_\xi(x_j)\big)^2 + U(x) + H_f. \qquad (2)$$

Here, $\kappa =$ particle charge, $U(x) =$ total potenial,

$A_\xi(y) =$ UV-regularized quantized vector potenial and

$H_f =$ photon Hamiltonian.

Infrared problem: infinite # of massless photons.

Qns: Emission and absorption of EM radiat., mass renormalization

Thm. Assume that $\langle\psi_t, N_{\mathrm{ph}}\psi_t\rangle \le C < \infty$ (satisfied in spec. cases). Then the asymptotic completeness holds.

Open problem: Prove $\langle\psi_t, N_{\mathrm{ph}}\psi_t\rangle \le C < \infty$ for general particle

Effective (Hartree and Hartree-Fock) Equations

Consider a system of n identical bosons or fermions with the Schrödinger equation

$$i\partial_t \psi = H_n \psi. \tag{SE}$$

To obtain an effective approximation for large n, we restrict the SE to the Hartree and Hartree-Fock states

$$\otimes_1^n \psi \quad \text{and} \quad \wedge_1^n \psi_i \tag{3}$$

This gives equations for ψ and $\psi_1, \ldots, \psi_n$ - the Hartree and Hartree-Fock equations, widely used in physics and chemistry.

However, the H and HF equations fail to describe quantum fluids: superconductors, superfluids and BE condensates. For this, one needs another conceptual step.

Non-Abelian random Gaussian fields and Wick states

We think of Hartree-Fock (HF) states as a non-Abelian generalization of random Gaussian fields uniquely determined by the two-point correlations:

$$\langle \psi^*(y)\, \psi(x) \rangle_t. \tag{4}$$

However, the above states are not the most general 'quadratic' states. The most general ones are defined by all two-point correlations

$$\langle \psi^*(y)\, \psi(x) \rangle_t \quad \text{and} \quad \langle \psi(x)\, \psi(y) \rangle_t. \tag{5}$$

This type of states were introduced by Bardeen-Cooper-Schrieffer for fermions and by Bogolubov, for bosons.

For such states all correlations are either 0 or are sums of products of quadratic ones (Wick property from QFT $\Longrightarrow$ Wick states).

They give the most general one-body approximation to the $n-$body dynamics.

Dynamics

Restricting the Schrödinger evolution to Wick states yields a system of coupled nonlinear PDE's for the functions

$$\begin{aligned}
&\phi(x,t) := \langle \psi(x) \rangle_t, \\
&\gamma(x,y,t) := \langle \psi^*(y)\, \psi(x) \rangle_t, \\
&\alpha(x,y,t) := \langle \psi(x)\, \psi(y) \rangle_t.
\end{aligned}$$

$\Longrightarrow$ The (time-dependent) *Bogolubov-de Gennes* (fermions)

and *Hartree-Fock-Bogolubov* (bosons) equations.

For the BEC: ϕ is the wave function of the BE condensate and

$\gamma(x,y,t)$ and $\alpha(x,y,t)$, viewed as the the integral kernels, yield the density operator γ of the non-condensed atoms and the 'pair operator' α for the superfluid component.

Hartree-Fock-Bogolubov system

Neglecting the α-component and taking $v = \lambda\delta$, $\lambda \in \mathbb{R}$ for the pair interaction potential, the HFB syst becomes (2−gas model)

$$i\partial_t\phi = h\phi + \lambda|\phi|^2\phi + 2\lambda\rho_\gamma\phi, \tag{GP}$$

$$i\partial_t\gamma = [h_{\gamma,\phi}, \gamma], \tag{HF}$$

where $h = -\Delta + V$ is a one-part. Schrödinger opr, and

$$h_{\gamma,\phi} := h + 2\lambda(\rho_\gamma + |\phi|^2),\ \rho_\gamma(x,t) := \gamma(x;x,t).$$

These are coupled Gross-Pitaevskii and Hartree-Fock equations

Problems: Existence, Ground st., Condensation, Collapse oscillat. for $\lambda < 0$ (correction to the Papanicolaou-Sulem[2] collapse law?).

Set-ups: External potentials vs translational invariance.

Bogolubov-de Gennes system

For fermions, $\phi(x,t) := \varphi_t(\psi(x)) = 0$ and, since the Wick states describe superconductors, (γ, α) are coupled to the EM field. Let a be the magnetic potential and take the gauge $\phi_{\mathrm{electr}} = 0$. Then

$$\begin{aligned} i\partial_t \gamma &= [h_{a,\gamma}, \gamma]_- + \dots, \\ i\partial_t \alpha &= [h_{a,\gamma}, \alpha]_+ + \dots, \\ -\partial_t^2 a &= \mathrm{curl}^* \,\mathrm{curl}\, a - j(\gamma, a), \end{aligned} \tag{BdG}$$

where $j(\gamma, a)(x) := [-i\nabla_a, \gamma]_+(x,x)$, the current density,

$$h_{a,\gamma} = -\Delta_a + g_{\mathrm{xc}}(\gamma), \tag{6}$$

with $\Delta_a := (\nabla + ia)^2$, and $[A,B]_\pm = AB^* \pm BA^*$.

These are the celebrated Bogolubov-de Gennes equations. They give the 'mean-field' (BCS) theory of superconductivity.

Key problem: Existence and stability of the ground/equillibrium state - static solution minimizing the free energy locally.

Gauge (magnetic) translational invariance

For the ground state (GS), look for the most symmetric state(s).

The BdG eqs are invariant under the (t-indep.) *gauge* transforms

$$T_\chi^{\text{gauge}} : (\gamma, \alpha, a) \to (e^{i\chi}\gamma e^{-i\chi}, e^{i\chi}\alpha e^{i\chi}, a + \nabla\chi) \qquad (7)$$

The simplest class of states: translationally invariant states for $a = 0$ and the gauge-translationally invariant ones for $a \neq 0$.

Gauge (magnetically) transl. invariant states are invariant under

$$T_{bs} : (\gamma, \alpha, a) \to (T_{\chi_s}^{\text{gauge}})^{-1} T_s^{\text{transl}}(\gamma, \alpha, a),$$

for any $s \in \mathbb{R}^d$. For $d = 2$, $\chi_s(x) := \frac{b}{2}(s \wedge x)$ (in a special gauge).

Here T_s^{transl}, $s \in \mathbb{R}^d$, is the group of translations and $b > 0$ is a parameter identified with a constant external magnetic field.

Ground State

Usually, the ground state (GS) has the max. symmetry $\Rightarrow$

Depending on the magnetic field b, one expects:

GS is translationally invariant for $b = 0$,

GS is the magnetically translationally invariant for $b \neq 0$.

Candidates for the ground state:

1. Normal states: (γ, α, a), with $\alpha = 0$ ($\Rightarrow \gamma$ is 'Gibbs state').
2. Superconducting states: (γ, α, a), with $\alpha \neq 0$ and $a = 0$.

Theorem (Hainzl-Hamza-Seiringer-Solovej). For $b = 0$, $\exists$ superconducting, normal, translationally invariant solution.

Theorem (CS). For $b \neq 0$, MT-invariance $\Longrightarrow$ normality ($\alpha = 0$).

Corollary. For $b \neq 0$, superconductivity $\Longrightarrow$ symmetry breaking.

Vortex lattices

For the GS, look for states with minimal symmetry breaking $\Longrightarrow$

- Vortex lattice: $T_s^{\mathrm{transl}}(\gamma, \alpha, a) = T_{\chi_s}^{\mathrm{gauge}}(\gamma, \alpha, a)$, $\forall s \in \mathcal{L}$ (some lattice in $\mathbb{R}^2$), a map $\chi_s : \mathcal{L} \times \mathbb{R}^2 \to \mathbb{R}$, and
  $\alpha \neq 0$.

T_s^{transl} is a group representation $\Longrightarrow$ χ_s satisfies the co-cycle relat:

$$\chi_{s+t}(x) - \chi_s(x+t) - \chi_t(x) \in 2\pi\mathbb{Z}, \;\; \forall s, t \in \mathcal{L}. \qquad (8)$$

Co-cycle relation (8) $\Longrightarrow$ the magnetic flux is quantized:

$$\frac{1}{2\pi} \int_{\Omega^{\mathcal{L}}} \operatorname{curl} a = c_1(\chi) \in \mathbb{Z}.$$

Here $\Omega^{\mathcal{L}}$ is a fundamental cell of $\mathcal{L}$ and $c_1(\chi)$ is the 1st Chern $\#$.

Existence of vortex lattices

Theorem. For the BdG syst without the self-interact. term:

(i) $\forall n$, $T > 0$ and $\mathcal{L}$ $\exists$ a static solution $u_{Tn\mathcal{L}} := (\gamma, \alpha, a)$ satisfying

$$u_{Tn\mathcal{L}} \text{ is } \mathcal{L}\text{-equivariant:} \quad T_s^{\mathrm{transl}} u_{Tn\mathcal{L}} = T_{\chi_s}^{\mathrm{gauge}} u_{Tn\mathcal{L}}, \forall s \in \mathcal{L}, \quad (9)$$

$$\text{1st Chern number is } n: \quad \int_{\Omega^{\mathcal{L}}} \mathrm{curl}\, a = 2\pi n, \quad (10)$$

$u_{nT\mathcal{L}}$ minimizes the free energy $F_T = E - TS$ on $\Omega^{\mathcal{L}}$ for $c_1 = n$;

(ii) For the pair potential $v \leq 0, v \not\equiv 0$ and T and b sufficiently small, $u_{Tn\mathcal{L}}$ is a vortex lattice (i.e. $\alpha \neq 0$);

(iii) For $n > 1$, there is a finer lattice, $\mathcal{L}' \supset \mathcal{L}$ for which $u_{Tn\mathcal{L}} = u_{T1\mathcal{L}'}$, i.e. $u_{Tn\mathcal{L}}$ is $\mathcal{L}'$-equivariant with $c_1 = 1$.

Ginzburg-Landau equations

In the leading approximation (close to the critical temperature and after 'integrating out' γ), the BdG system leads to the *time-dependent Ginzburg-Landau equations*

$$\gamma\partial_t\psi = \Delta_a\psi + \kappa^2(1-|\psi|^2)\psi,$$
$$\nu\partial_t a = -\operatorname{curl}^2 a + \operatorname{Im}(\bar{\psi}\nabla_a\psi),$$

in the gauge $\phi_{\mathrm{electr}} = 0$, where $\operatorname{Re}\gamma, \operatorname{Re}\nu \geq 0$. Interpretations:

> $|\psi|^2$ is the density of superconducting electrons;
> $a : \mathbb{R}^{d+1} \to \mathbb{R}^d$ is the magnetic potential;
> $\operatorname{Im}(\bar{\psi}\nabla_a\psi)$ is the superconducting current.

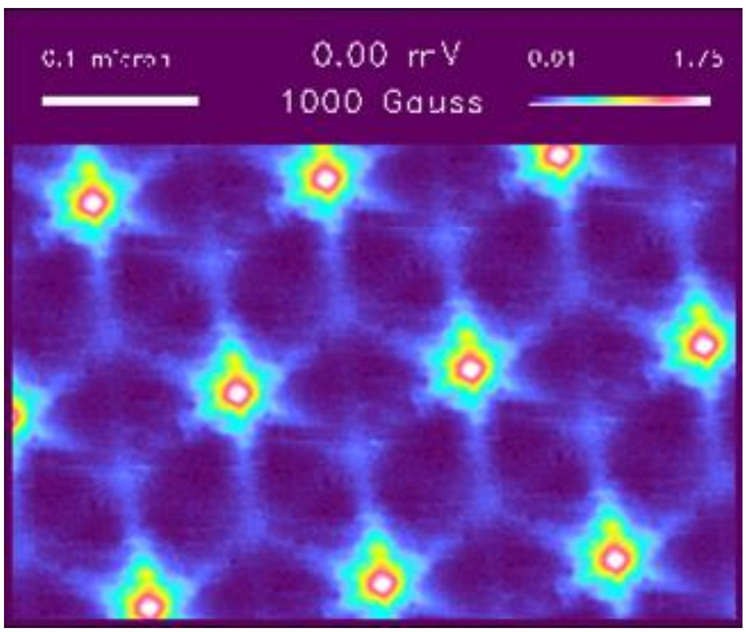
The last equation comes from two Maxwell equations (Ampère's and Faraday's laws).

GLE: Ground state

Major open problem:

- Structure of the ground state (vortex lattice?) and its stability

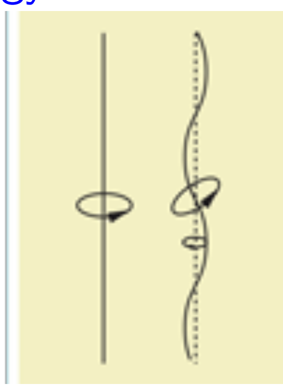
Experiment: the ground state is the hexagonal vortex lattice.

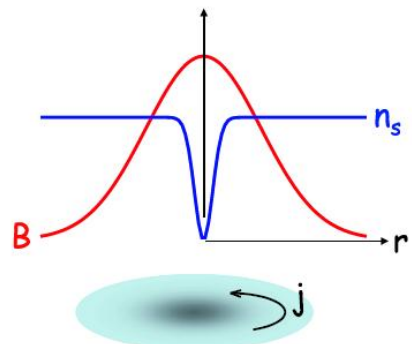


Theoretical description: the BdG system with the coarse-scale approximation given by the Ginzburg-Landau system.

GLE: vortex lattices

A vortex lattice solution is formed by magnetic vortices (localized finite energy solutions of a fixed degree),





arranged in a (mesoscopic) lattice $\mathcal{L}$.

The existence of vortex lattices (VL) for the GLE (and now for BdG) and their energetic properties (for GLE) are well understood.

Since the VL are not localized, the stability is a delicate matter.

Thm: The vortex lattices are stable under lattice-periodic and local perturbations.

Question: Stability under more general lattice deformations?

References

n−particle scattering: Soffer-IMS ($\mu > 1$), Dereziński ($\mu > \sqrt{3} - 1$); Deift, Gérard, Graf, Mourre, Simon, Yafaev, et al

NR QED, radiation: Bach-Fröhlich-IMS, Griesemer-Lieb-Loss, Hasler-Herbst, Th. Chen, Hübner-Spohn, Skibsted, Møller, Pizzo, Hiroshima, Hainzl-Seiringer, Teufel, Faupin, A. Panati, Miyao, et al

NR QED, Asymptotic completeness: Faupin-IMS, De Roeck-Griesemer-Kupiainen; Spohn, Dereziński-Gérard, Fröhlich-Griesemer-Schlein, Griesemer-Zenk, Dybalski-Pizzo, et al

HFB: Bach-Breteaux-Chen-Fröhlich-IMS, Napiórkoswki-Reuvers-Solovej et al.

BdG w/ $a = 0$: Frank, Hainzl, Seiringer, Benedikter-Sok-Solovej, ...

Existence of vortex lattices for BdG: Chenn-IMS

Stability of vortex lattices for GL: Tzaneteas-IMS

Summary

- We reviewed some basic properties of the Schrödinger eq which encodes all the information about quantum systems.
- While we learned much about the general structure of this equation, our understanding of specific quantum systems with the number of particles ≥ 3 is spotty and progress, with some notable exceptions like the stability of matter, is very slow.
- However, there is one important direction where robust progress is possible - 'effective' equations for quantum systems of large number of identical particles, especially, superconductors, superfluids and Bose-Einstein condensates - the HFB and BdG eqs.
- Important area not touched in this talk: DFT.

Thank-you for your attention