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 $\psi = \psi(x_1, \dots, x_n, t)$ 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 & unitar.$\Longleftrightarrow$ self-adjointness of H_n

Goal: Describe the space-time behaviour of solutions

Main problem: *stability vs break-up or collapse.*

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

- *stability w. r. to collapse* ($\inf H_n > -\infty$)
- *stability w. r. to break-up* ($\inf H_n =$ *eigenvalue*).

Break-up (Local decay) $\Longrightarrow$ *scattering*

Scattering

The main mathematical problem of the scattering theory

Asymptotic completeness: 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 (Soffer-IMS ($\mu > 1$), Dereziński ($\mu > \sqrt{3} - 1$))

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.

Earlier works: Deift, Enss, Gérard, Graf, Mourre, Simon, Yafaev, ...

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 potential, $H_f =$ photon Hamiltn.

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

Infrared problem: photons $\Longrightarrow$ infinite clouds of gapless 'excitations'.

Main qstn: Math. descript. of the processes of emiss. and absorp. of rad.

Bach-Fröhlich-IMS: stability of the *ground state* and instability of the *excited states* of the particle system (say, an atom)
and emergence of resonances.

Further results: Th. Chen, Griesemer-Lieb-Loss, Hasler-Herbst, Hiroshima, Hainzl-Seiringer, Hübner-Spohn, Miyao, Møller, A. Panati, Pizzo, Teufel, et al

Scattering

Consider the Rayleigh scattering, i.e. the scattering at the energy $<$ the ionization energy of atomic or molecular system.

Thm (Faupin-IMS, De Roeck-Griesemer-Kupiainen). Assume that

$$\langle \psi_t, N_{\rm ph} \psi_t \rangle \le C < \infty \quad \text{(satisfied in spec. cases[1])}.$$

Then the asymptotic completeness holds.

Earlier results: Spohn, Dereziński-Gérard, Fröhlich-Griesemer-Schlein, et al

Open problem: Prove $\langle \psi_t, N_{\rm ph} \psi_t \rangle \le C < \infty$ for general particle systems (like atoms).

[1] De Roeck-Kupiainen, spin-boson model, Faupin-IMS, some generalizations

Effective (Hartree and Hartree-Fock) Equations

Effective equations is a powerful tool in study of complex systems. For the n-particle quantum systems, a key effective equation is the Hartree-Fock equation

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

where γ is a (trace class) positive operator (density opr) and h_γ is the self-consistent Hamiltonian:

$$h_\gamma := -\Delta + V + g(\gamma),$$

with the self-interaction energy $g(\gamma) = v \star \rho_\gamma + ex_{\mathrm{HF}}(\gamma)$. Here

$$\rho_\gamma(x,t) := \gamma(x;x,t) \qquad \text{(charge density)}.$$

For fermions $\gamma \leq \mathbf{1}$, for bosons, $\gamma < \infty$ and $ex_{\mathrm{HF}} = 0$

The HF eq trades the degrees of freedom for nonlinearity. It is widely used in quantum chemistry and condensed matter physics.

Density functional theory

Replacing the the exchange term, $ex_{\mathrm{HF}}(\gamma)$, in the HF eq by a function $xc(\rho_\gamma)$ (exchange and correlation energy) of the 1-particle (charge) density ρ_γ (LDA), one arrives at the (t-dep) Kohn-Sham equation

$$i\partial_t\gamma = [h_{\rho_\gamma}, \gamma], \tag{KS}$$

$$h_\rho := -\Delta + v * \rho + xc(\rho) \quad \text{(self-consist ham)}, \tag{SCH}$$

$$\rho_\gamma(x,t) := \gamma(x;x,t) \qquad \text{(charge density)}. \tag{CD}$$

Density functional theory (DFT): Runge-Gross (modelled on Hochenberg-Kohn and Levy-Lieb theories): under certain conditions,

$$\exists xc(\rho): \qquad i\partial_t\Psi = H_n\Psi \Longrightarrow \gamma := \mathrm{Tr}_{(n-1)} P_\Psi \text{ satisfies (KS).}$$

Quant Chem./Cond. Matt. Phys. : Design $xc(\rho)$ depending on model.

Pusateri-IMS: Short-range scatt. $|xc(\rho)| \lesssim \rho^\beta, \beta > 1/\min(d,2)$

Open problem: Long-range scattering

Earlier results: Reduced HF eq ($xc = 0$): Stability of ground states (Lewin-Sabin, Th. Chen-Pavlovic)

Quantum liquids

However, the H and HF equations fail to describe quantum matter at nano- and macro-scales: superconductors, superfluids and BE condensates. For this, one needs another conceptual step:

Pass to the most general quasi-free (one-body) approximation to the $n-$body dynamics, of which the HF approximation is a special case.

Such a step was made by Bardeen-Cooper-Schrieffer for fermions and by Bogolubov, for bosons, and resulted in[2]

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

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

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Key problem: Existence and stability of the ground/equilibrium state - static solution minimizing the free energy (locally, for translation invariance) $\Longrightarrow$ symmetry breaking.

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[2]See Bach-Bret-Chen-Fröhl-IMS, Chenn-IMS, Benedicter-Sok-Solovej

Hartree-Fock-Bogolubov system[3]

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)

$$i\partial_t \phi = h\phi + \lambda|\phi|^2\phi + 2\lambda\rho_\gamma\phi, \qquad \text{(GP)}$$
$$i\partial_t \gamma = [h_{\gamma,\phi}, \gamma], \qquad \text{(HF)}$$

where $h = -\Delta + V$ is a one-part. Schrödinger opr, $\rho_\gamma(x,t) := \gamma(x;x,t)$,

$$h_{\gamma,\phi} := h + 2\lambda(\rho_\gamma + |\phi|^2). \qquad \text{(scSO)}$$

These are coupled Gross-Pitaevskii and Hartree-Fock equations

Here the condensate of atoms (ϕ) is coupled to a cloud of the thermal atoms (γ).

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

Partial results of transl. invar. case: NapiorkowskiReuvSol, BBCF

[3] See Bach-Breteaux-Chen-Fröhlich-IMS

Bogolubov-de Gennes system

For fermions (electrons), (γ, α) couple to the EM field. Let a be the magnetic potential and take the gauge $\phi_{\mathrm{electr}} = 0$. Then[4]

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

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

$$h_{a,\gamma} = -\Delta_a + g_{\mathrm{xc}}(\gamma), \tag{3}$$

with $\Delta_a := (\nabla + ia)^2$, and $[A, B]_+ = AB + B\bar{A}$, $\bar{A} := \mathcal{C}A\mathcal{C}$.

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

Key problem: Existence of the ground/equillibrium state (static soln minimizing the free energy locally) and symmetry breaking?

[4] Chenn-IMS, Benedicter-Sok-Solovej

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

$$T_\chi^{\mathrm{gauge}} : (\gamma, \alpha, a) \to (e^{i\chi}\gamma e^{-i\chi}, e^{i\chi}\alpha e^{i\chi}, a + \nabla\chi) \qquad (4)$$

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

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

for any $s \in \mathbb{R}^d$. For $d = 2, 3$, $\chi_s(x) := \frac{b}{2} \cdot (s \wedge x)$ (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 magnetically translationally (MT) invariant for $b \neq 0$.

Candidates for the ground state:

1. Normal states: (γ, α, a), with $\alpha = 0$ ($\Rightarrow \gamma$ is Fermi-Dirac 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 (Chenn-IMS). 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: $\exists$ lattice $\mathcal{L}$ in $\mathbb{R}^2$ and map $\chi_s : \mathcal{L} \times \mathbb{R}^2 \to \mathbb{R}$:

$$T_s^{\mathrm{transl}}(\gamma, \alpha, a) = T_{\chi_s}^{\mathrm{gauge}}(\gamma, \alpha, a), \ \forall s \in \mathcal{L}, \text{ and } \alpha \neq 0.$$

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

$$\chi_{s+t}(x) - \chi_s(x+t) - \chi_t(x) = \frac{b}{2} \cdot (s \wedge t) \in 2\pi\mathbb{Z}, \ \forall s, t \in \mathcal{L}. \tag{5}$$

Co-cycle relation (5) $\Longrightarrow$ the magnetic flux is quantized:

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

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

$$u_{Tn\mathcal{L}} \text{ is } \mathcal{L}\text{-equivariant:} \quad T_s^{\mathrm{transl}} u_{Tn\mathcal{L}} = T_{\chi_s}^{\mathrm{gauge}} u_{Tn\mathcal{L}}, \forall s \in \mathcal{L}, \tag{6}$$

$$\text{1st Chern number is } n: \quad \int_{\Omega^{\mathcal{L}}} \operatorname{curl} a = 2\pi n, \tag{7}$$

$u_{nT\mathcal{L}}$ 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 $c_1 = 1$.

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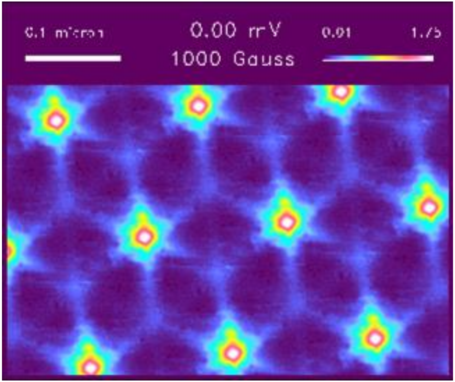
Remark: (ii) $\Longrightarrow$ Symmetry breaking in the ground state

Open problem: Is the vortex lattice a ground state?

Global minimizer (locally) vs emerging local minimizer.

Experiment

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

$$\Delta_a \psi + \kappa^2 (1 - |\psi|^2)\psi = 0,$$

$$-\operatorname{curl}^2 a + \operatorname{Im}(\bar{\psi} \nabla_a \psi) = 0.$$

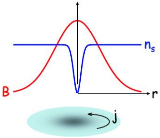
($|\psi|^2$ is the density of superconducting electrons)

Ginzburg-Landau equations: vortex lattices

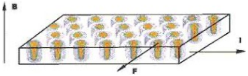
Thm: For type II superconductors ($\kappa > 1/\sqrt{2}$), $\exists b_*$ s.t. for $b > b_*$, the homogeneous soln, u_b^{hom}, with the constant magnetic field b, is a local minimizer of $E_{\mathrm{GL}}(u)$ and for $b < b_*$, it is not.

$\forall b < b_*$ and lattice $\mathcal{L}$, $\exists$ a soln, $u_b^{\mathcal{L}}$, with the lattice $\mathcal{L}$ symmetry, with

$$\frac{1}{2\pi}\int_{\Omega^{\mathcal{L}}} \mathrm{curl}\, a = b, \quad \text{and} \quad E_{\mathrm{GL}}(u^{\mathcal{L}}) < E_{\mathrm{GL}}(u^{\mathrm{hom}}).$$



Thm(Tzanet-IMS): Soln $u_b^{\mathcal{L}}$ is formed by magn. vortices

arranged in a lattice $\mathcal{L}$. 

Thm (Tzanet-IMS): Vort. lattices are local minima of the GL energy w.r.to (i.e. stable under) period & local perts.

Problem: Stability under more general lattice deformations?
Discussion: Global minimizer (locally) vs bifurcation of local minimizer?

Summary

We reviewed some results on quantum many-particle problem:

- *n*-particle scattering
- interaction of radiation and matter
- effective equations for quantum gases and quantum liquids (HF, KS-DFT, HFB, BdG, GL equations)

I highlighted a number of basic open problems in these central areas of quantum mechanics. They concentrated on

- Long-time behaviour
- Existence and stability of ground states
- Symmetry breaking

Thank-you for your attention