Marco Falconi
Università di Roma Tre
mfalconi@mat.uniroma3.it

Variational Problems in Quasi-Classical Systems

(Joint work with M. Correggi and M. Olivieri)

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Force-Carriers in quantum systems at low- and medium- energy scales

- **Force-Carriers**
  - The fundamental forces of the standard model are carried by bosonic fields (photons, $W^{\pm}$ and Z bosons, gluons).
  - Any reasonable quantization of gravity would also result in a bosonic field (gravitons).
  - Collective excitations in many-body quantum mechanics (phonons, magnons, plasmons, rotons,…) are also described by bosonic fields.
- **Low- and medium- energy scales**
  - At low- and medium- energy scales, the quantum nature of the force-carrying fields does not play an important role.
  - Photons, phonons, gravitons behave, in very good approximation, as classical force fields: electromagnetic, vibrational, and gravitational, respectively.

The energy of a coupled "particles – force carrier" system

- $$E = \langle \Psi, H\Psi \rangle$$
- $$H = \underbrace{\sum_{j=1}^{N} -\Delta_j + V(x_1, \dots, x_N)}_{\text{particles}} + \underbrace{\int \omega(k) a^*(k) a(k)}_{\text{force carrier}} + \underbrace{H_{\mathrm{I}}(x, -i\nabla, a, a^*)}_{\text{interaction}}$$

The energy of a coupled "particles – force carrier" system at low- and medium- energy scales

- $$E_\varepsilon = \langle \Psi_\varepsilon, H_\varepsilon \Psi_\varepsilon \rangle$$

- $$H_\varepsilon = \underbrace{\sum_{j=1}^{N} -\Delta_j + V(x_1, \dots, x_N)}_{\text{particles}} + \underbrace{\int \omega(k) a_\varepsilon^*(k) a_\varepsilon(k)}_{\text{force carrier}} + \underbrace{H_{\mathrm{I}}(x, -i\nabla, a_\varepsilon, a_\varepsilon^*)}_{\text{interaction}}$$

- $$[a_\varepsilon(k), a_\varepsilon^*(k')] = \varepsilon \delta(k - k') \ .$$

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- $$\boxed{H_\varepsilon = \underbrace{\sum_{j=1}^{N} -\Delta_j + V(x_1, \dots, x_N)}_{\text{particles}} + \underbrace{\mathrm{Op}_\varepsilon^{\mathrm{Wick}}(\mathcal{F}(z, \bar{z}))}_{\substack{\text{force carrier} \\ \text{(quasi-classical)}}} + \underbrace{\mathrm{Op}_\varepsilon^{\mathrm{Wick}}(\mathcal{H}_{\mathrm{I}}(x, -i\nabla, z, \bar{z}))}_{\substack{\text{interaction} \\ \text{(quasi-classical)}}}}$$

- $$[a_\varepsilon(k), a_\varepsilon^*(k')] = \varepsilon \delta(k - k') .$$

Explicit models considered

- **Nelson:**

$$H_\varepsilon = -\Delta + V + \int_{\mathbb{R}^d} \omega(k) a_\varepsilon^*(k) a_\varepsilon(k) + a_\varepsilon(\lambda_x) + a_\varepsilon^*(\lambda_x) \ .$$

- **Polaron:**

$$H_\varepsilon = -\Delta + V + \int_{\mathbb{R}^3} a_\varepsilon^*(k) a_\varepsilon(k) + a_\varepsilon(\pi_x) + a_\varepsilon^*(\pi_x) \ .$$

- **Pauli-Fierz:**

$$H_\varepsilon = \Big(-i\nabla + eA_\varepsilon(x)\Big)^2 + V + \sum_{\mu=1}^{d-1} \int_{\mathbb{R}^d} |k| a_{\varepsilon,\mu}^*(k) a_{\varepsilon,\mu}(k) \ .$$

Explicit models considered

- **Nelson:**

$$H_\varepsilon = -\Delta + V + \mathrm{Op}_\varepsilon^{\mathrm{Wick}}\big(\langle z, \omega z\rangle_{\mathfrak{h}}\big) + \mathrm{Op}_\varepsilon^{\mathrm{Wick}}\big(2\mathfrak{R}\langle \lambda_x, z\rangle_{\mathfrak{h}}\big) .$$

- **Polaron:**

$$H_\varepsilon = -\Delta + V + \mathrm{Op}_\varepsilon^{\mathrm{Wick}}\big(\|z\|_{\mathfrak{h}}^2\big) + \mathrm{Op}_\varepsilon^{\mathrm{Wick}}\big(2\mathfrak{R}\langle \underbrace{\pi_x}_{\notin \mathfrak{h}}, z\rangle_{\mathfrak{h}}\big) .$$

- **Pauli-Fierz:**

$$H_\varepsilon = \Big(-i\nabla + e\,\mathrm{Op}_\varepsilon^{\mathrm{Wick}}\big(A(x,z,\bar{z})\big)\Big)^2 + V + \sum_{\mu=1}^{d-1} \mathrm{Op}_\varepsilon^{\mathrm{Wick}}\big(\langle z_\mu, |\cdot| z_\mu\rangle_{\mathfrak{h}}\big) .$$

Quasi-Classical Limit $\varepsilon \to 0$

- How does the system behave, at leading order, at low- and medium-energy scales?
- In other words, does E_ε have a limit as $\varepsilon \to 0$? If so, can we characterize the limit more or less explicitly?
- We are able to provide a satisfactory answer if we consider the ground state energy

$$e_\varepsilon = \inf_{\|\Psi_\varepsilon\|=1} E_\varepsilon = \inf_{\|\Psi_\varepsilon\|=1} \langle \Psi_\varepsilon, H_\varepsilon \Psi_\varepsilon \rangle ,$$

as well as the corresponding ground states/minimizing sequences.

Quasi-Classical Energy

- $$\mathcal{E}(\psi, z) = \left\langle \psi , \left(-\Delta + V(x) + \mathcal{H}_I(x, -i\nabla, z, \bar{z}) \right) \psi \right\rangle + \mathcal{F}(z, \bar{z}) \, .$$
- $$e_0 = \inf_{\substack{(\psi,z) \\ \|\psi\|=1}} \mathcal{E}(\psi, z) \, .$$

Remark

As we will discuss shortly, the quasi-classical energy approximates well the ground state energy of the system. However, it *shall not* be seen as the Hamiltonian generating the quasi-classical dynamics: the latter is in fact *non-Hamiltonian*.

- In some cases it is of interest to carry out the minimization with respect to the classical field beforehand, obtaining thus an effective (nonlinear) energy for the quantum subsystem:

$$\boxed{E_0(\psi) = \inf_z \mathcal{E}(\psi, z)\ ;}$$

$$\boxed{\varepsilon_0 = \inf_{\|\psi\|=1} E_0(\psi)\ .}$$

  - **Typical example:** For the polaron model, E_0 is the Pekar energy functional

$$E_0(\psi) = \langle \psi, (-\Delta + V)\psi \rangle - \int_{\mathbb{R}^6} \frac{|\psi(x)|^2 |\psi(y)|^2}{|x-y|} \mathrm{d}x \mathrm{d}y\ .$$

  - In other cases, such as the Pauli-Fierz model, the nonlinearity in E_0 may not be explicitly definable.

Convergence of the Ground State Energy

Theorem (CFO20)

$$\lim_{\varepsilon \to 0} e_{\varepsilon} = e_0 = \varepsilon_0 \, .$$

Quasi-Classical States

- What is the quasi-classical limit $\varepsilon \to 0$ of a pure state

$$|\Psi_\varepsilon\rangle\langle\Psi_\varepsilon| \,,$$

  or more generally of a density matrix

$$\Gamma_\varepsilon \, ?$$

- Under suitable assumptions[1], the limit is a *state-valued measure*:

$$\underbrace{\gamma(z)}_{\text{density matrix for the quantum subsystem}} \; \overbrace{\mathrm{d}\mu(z)}^{\text{measure on the space of classical configurations } \mathfrak{h}}$$

[1] $\mathrm{Tr}(\Gamma_\varepsilon(\int a_\varepsilon^*(k) a_\varepsilon(k))^\delta) \leq C$

- More precisely, let $(\Gamma_\varepsilon)_{\varepsilon\in(0,1)}$ be a family of density matrices such that there exist $\delta > 0$ and $C > 0$ such that

$$\mathrm{Tr}\big(\Gamma_\varepsilon \mathcal{N}_\varepsilon^\delta\big) \leq C \,.$$

Then there exists a sequence $\varepsilon_n \to 0$ and a state-valued measure $\gamma(z)\mathrm{d}\mu(z)$ (called a *Wigner measure* of Γ_ε) such that

$$\boxed{\Gamma_{\varepsilon_n} \underset{n\to\infty}{\longrightarrow} \gamma(z)\mathrm{d}\mu(z) \,.}$$

- ⚠ :

$$\boxed{0 \leq \mu(\mathfrak{h}) \leq 1 \,.}$$

- The convergence above is intended as follows: for nice enough "symbols" $f(x, -i\nabla, z)$,

$$\boxed{\lim_{n\to\infty} \mathrm{Tr}\Big(\Gamma_{\varepsilon_n} \mathrm{Op}_{\varepsilon_n}^{\mathrm{Wick}}\big(f(x,-i\nabla,z)\big)\Big) = \int_{\mathfrak{h}} \mathrm{tr}\Big(\gamma(z) f(x,-i\nabla,z)\Big)\mathrm{d}\mu(z) \,.}$$

Quasi-Classical Minimizing Sequences

- Let us now consider a minimizing sequence $|\Psi_\varepsilon\rangle\langle\Psi_\varepsilon|$ for e_ε, such that

$$\boxed{\langle\Psi_\varepsilon, H_\varepsilon\Psi_\varepsilon\rangle < e_\varepsilon + \varepsilon\,.}$$

  Does this family qualify as a quasi-classical state? Are its corresponding Wigner measures “well-behaved”?

- The answers are both yes, *as long as the quantum subsystem is confined*.
- If the quantum subsystem is not confined, the state-valued is not as well behaved, in particular the $\gamma(z)$ in that case would not be, roughly speaking, a density matrix[2].

[2] In this case the natural target space for the Wigner measures would be that of generalized quantum states, in the algebraic sense; still the result is crucial to prove the convergence of the ground state energy in the unconfined case

Confined Case

- Confinement in the quantum part amounts to choosing V in H_ε such that $\lim_{|x|\to+\infty} V(x) = +\infty$.
- Confinement guarantees that:
  - If $\gamma(z)\mathrm{d}\mu(z)$ is a Wigner measure of $|\Psi_\varepsilon\rangle\langle\Psi_\varepsilon|$, then μ is a *probability measure*.
- The uniform expectation of an arbitrary power of the number operator is guaranteed, in the models considered, by the fact that Ψ_ε is a minimizing sequence and that e_ε is finite (*i.e.* H_ε is bounded from below). Therefore, at least one Wigner measure of $|\Psi_\varepsilon\rangle\langle\Psi_\varepsilon|$ exists.

- Analogously, it is guaranteed that if $|\Psi_{\varepsilon_n}\rangle\langle\Psi_{\varepsilon_n}| \longrightarrow \gamma(z)\mathrm{d}\mu(z)$, then, for the models considered,

$$\lim_{n\to\infty}\langle\Psi_{\varepsilon_n}, (-\Delta + V + H_I)\Psi_{\varepsilon_n}\rangle = \int_{\mathfrak{h}} \mathrm{tr}\Big(\gamma(z)(-\Delta + V + \mathscr{H}_I(z))\Big)\mathrm{d}\mu(z)\,;$$

and

$$\int_{\mathfrak{h}}\Big(\mathrm{tr}\Big(\gamma(z)(-\Delta + V + \mathscr{H}_I(z))\Big) + \mathscr{F}(z)\Big)\mathrm{d}\mu(z) < +\infty\,.$$

- ⚠ : The limit

$$\lim_{n\to\infty}\langle\Psi_{\varepsilon_n}, \mathrm{Op}^{\mathrm{Wick}}_{\varepsilon_n}(\mathscr{F}(z))\Psi_{\varepsilon_n}\rangle$$

could differ from

$$\int_{\mathfrak{h}} \mathscr{F}(z)\mathrm{d}\mu(z)\,!$$

This is a loss of compactness phenomenon due to the fact that $\mathfrak{h}$ is infinite dimensional.

- Still it is possible to approximate $\mathscr{F}(z)$ from below with a symbol that does not have loss of compactness.
- In the end, one obtains that for any Wigner measure of $|\Psi_\varepsilon\rangle\langle\Psi_\varepsilon|$ (and at least one exists):

$$\int_{\mathfrak{h}} \Big(\mathrm{tr}\Big(\gamma(z)\big(-\Delta + V + \mathscr{H}_I(z)\big)\Big) + \mathscr{F}(z)\Big)\mathrm{d}\mu(z) \leq \liminf_{\varepsilon\to 0} e_\varepsilon \; (= e_0)\,.$$

- This provides two important pieces of information:
  - $$e_0 \leq \liminf_{\varepsilon\to 0} e_\varepsilon\,;$$

    hence one has the lower bound necessary to establish the convergence $e_\varepsilon \longrightarrow e_0$ (the upper bound is easy, using well-known trial functions);
  - $$\underset{(\psi,z)}{\mathrm{conv.\,comb.}}\Big[\mathcal{E}(\psi,z)\Big] = e_0\,.$$

- Therefore, *$\mathcal{E}$ has minimizers*, and the following theorem holds:

Theorem (CFO20)

In the trapped case, any Wigner measure of any minimizing sequence $(\Psi_\varepsilon)_{\varepsilon\in(0,1)}$ satisfying

$$\langle\Psi_\varepsilon, H_\varepsilon\Psi_\varepsilon\rangle < e_\varepsilon + \varepsilon$$

is concentrated on the nonempty set of minimizers of the quasi-classical energy functional $\mathcal{E}$.

Remarks

- If H_ε has a ground state(s), the above theorem clearly holds for it as well.
- If the minimizer $(\underline{\psi}, \underline{z})$ of $\mathcal{E}$ is unique, up to a global phase factor for $\underline{\psi}$, then

$$|\Psi_\varepsilon\rangle\langle\Psi_\varepsilon| \underset{\varepsilon\to 0}{\longrightarrow} |\underline{\psi}\rangle\langle\underline{\psi}|\, \mathrm{d}\delta(z-\underline{z})\,.$$

Thank you for the attention