The time-dependent Hartree-Fock-Bogoliubov equation for Bosons

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14-May-2018

1. Quantum-Mechanical Many-Body Problem
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Consider a system of many particles in $\mathbb{R}^d$, $d \in \mathbb{N}$.

- The one-particle Hilbert space is $\mathfrak{h} := L^2(\mathbb{R}^d)$.
- The Hilbert space of N particles is the subspace $\mathcal{F}^{(N)} := \mathcal{S}[\mathfrak{h}^{\otimes N}]$ of symmetric vectors in $\mathfrak{h}^{\otimes N}$.
- The Hamiltonian generating the dynamics of an N-particle system is

$$H^{(N)} := \sum_{n=1}^{N} h_n + \sum_{1 \le m < n \le N} v(x_m - x_n),$$

where $h_n := -\Delta_{x_n} + V(x_n)$ is the one-particle Hamiltonian, and $v(x-y)$ is the pair interaction potential.

To study states of all possible particle numbers $N \geq 0$ in a single vector, we pass to boson Fock space.

- The Hilbert space of many-particle states is the boson Fock space $\mathcal{F} := \bigoplus_{N=0}^{\infty} \mathcal{F}^{(N)}$.
- The Hamiltonian generating the dynamics of many-particle states is $\mathbb{H} := \bigoplus_{N=0}^{\infty} H^{(N)}$.
- It is convenient to represent the boson Fock space as $\mathcal{F} = \overline{\mathrm{span}\{\psi^*(f_1) \cdots \psi^*(f_N)\Omega \,|N \in \mathbb{N}_0, f_j \in \mathfrak{h}\}}$, where $\psi^*(f) = \int f(x)\, \psi(x)^*\, dx$ are the creation operators and $\Omega \in \mathcal{F}^{(0)}$ is the vacuum vector.
- Creation operators and their adjoints $\psi(f) := \big(\psi^*(f)\big)^*$, the annhiliation operators, fulfill the CCR $[\psi(x), \psi(y)] = [\psi^*(x), \psi^*(y)] = 0$, $[\psi(x), \psi^*(y)] = \delta(x - y)$, $\psi(x)\Omega = 0$, on $\mathcal{F}$.

On Fock space, all observables can be expressed in terms of creation and annihilation op's, e.g., $\mathbb{H} := \bigoplus_{N=0}^{\infty} H^{(N)}$ is

$$\mathbb{H} \; = \int \psi^*(x)\, [h\psi](x)\, dx + \frac{1}{2} \iint v(x-y)\, \psi^*(x)\, \psi^*(y)\, \psi(y)\, \psi(x)\, dx\, dy \,,$$

with $h = -\Delta + V(x)$. We assume either

(H) $V \ll -\Delta, \qquad v \ll -\Delta,\ v(x) = v(-x)$, or

(H') $V \ll -\Delta, \qquad \exists p > d:\ v \in W^{p,1}(\mathbb{R}^d),\ v(x) = v(-x)$.

- The dynamics is defined by the Schrödinger equation $i\partial_t \Psi(t) = \mathbb{H}\Psi(t)$, $\Psi_0 \in \mathcal{F}$.
- If $\rho_t = \sum_j \lambda_j |\Psi_j(t)\rangle\langle\Psi_j(t)| \in \mathcal{L}^1_+(\mathcal{F})$ is a density matrix, the Schrödinger equation for ρ_t reads $i\partial_t \rho_t \;=\; [\mathbb{H}, \rho_t]$.
- For quantum states $\mathbb{A} \mapsto \omega_t(\mathbb{A}) := \mathrm{Tr}\{\rho_t \mathbb{A}\}$, this is equivalent to the von Neumann-Landau equation,

$$i\partial_t \omega_t(\mathbb{A}) \;=\; \omega_t\big([\mathbb{A}, \mathbb{H}]\big) \,,$$

where $\mathbb{A} \in \mathcal{B}[\mathcal{F}]$ is an observable.

- Given a state ω, its one- and two-point functions are defined as

$$\begin{aligned} \phi_\omega(x) &:= \omega\big(\psi(x)\big), \\ \gamma_\omega(x,y) &:= \omega\big(\psi^*(y)\,\psi(x)\big) - \omega\big(\psi^*(y)\big)\omega\big(\psi(x)\big) \;=\; \omega\big(\eta^*(y)\,\eta(x)\big), \\ \sigma_\omega(x,y) &:= \omega\big(\psi(y)\,\psi(x)\big) - \omega\big(\psi(y)\big)\omega\big(\psi(x)\big) \;=\; \omega\big(\eta(y)\,\eta(x)\big), \end{aligned}$$

  where $\eta(x) := \psi(x) - \omega(\psi(x))$ and $\eta^\tau \in \{\eta, \eta^*\}$.
- A state ω is quasifree if all higher truncated correlation functions vanish, i.e., if $\omega\big(\eta^{\tau_1}(x_1)\cdots\eta^{\tau_{2k-1}}(x_{2k-1})\big) = 0$ and

$$\begin{aligned} &\omega\big(\eta^{\tau_1}(x_1)\cdots\eta^{\tau_{2k}}(x_{2k})\big) \\ &= \sum_{\pi\in\mathcal{P}_{2k}} \prod_{\nu=1}^{k} \omega\Big(\eta^{\tau_{\pi(2\nu-1)}}\big(x_{\pi(2\nu-1)}\big)\,\eta^{\tau_{\pi(2\nu)}}\big(x_{\pi(2\nu)}\big)\Big). \end{aligned}$$

- Quasifree states are the quantum analogue of Gaussian probability distributions.

- The von Neumann-Landau dynamics does not preserve quasifreeness, i.e., if ω_0^q is quasifree and ω_t is determined by $i\partial_t \omega_t(\mathbb{A}) = \omega_t\big([\mathbb{A}, \mathbb{H}]\big)$ then ω_t is not quasifree for $t > 0$.
- The (nonlinear) quasifree approximative dynamics ω_t^q for quasifree initial value ω_0^q is defined for $t > 0$ by demanding that (a) ω_t^q be quasifree and (b)

$$i\partial_t \omega_t^q(\mathbb{A}) \;=\; \omega_t^q\big([\mathbb{A}, \mathbb{H}]\big) \,,$$

  to hold true for all observables $\mathbb{A}$ that are linear or quadratic in $\psi^*(x)$ anbd $\psi(y)$.
- These requirements are equivalent to the HFB equation

$$i\partial_t \omega_t^q(\mathbb{A}) \;=\; \omega_t^q\big([\mathbb{A}, \mathbb{H}_{\mathrm{hfb}}(\omega_t^q)]\big) \,,$$

  for all observables $\mathbb{A}$ (of arbitrary degree), where $\mathbb{H}_{\mathrm{hfb}}(\omega_t^q)$ is the effective HFB Hamiltonian.

The HFB equation $i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q\big([\mathbb{A}, \mathbb{H}_{\rm hfb}(\omega_t^q)]\big)$ contains the effective HFB Hamiltonian

$$\begin{aligned} \mathbb{H}_{\rm hfb}(\omega^q) \; &= \int \psi^*(x)\,\big[h(\gamma)\psi\big](x)\,dx \\ &\quad - \int b\big[|\phi\rangle\langle\phi|\big]\,\phi(x)\,\psi^*(x) \\ &\quad + \frac{1}{2}\iint \big[v\#\sigma\big](x,y)\,\psi^*(x)\,\psi^*(y) + adj.\,, \end{aligned}$$

where $h(\gamma) := h + b[\gamma]$, $b[\gamma] := v * d(\gamma) + v\#\gamma$, $d(\gamma)(x) := \gamma(x,x)$, and $[v\#\gamma](x,y) := v(x-y)\sigma(x,y)$.

Since ω_t^q is determined by $\phi_t := \phi_{\omega_t^q}$, $\gamma_t := \gamma_{\omega_t^q}$, and $\sigma_t := \sigma_{\omega_t^q}$, the HFB equation is equivalent to the system

$$\begin{aligned} i\partial_t\phi_t &= h(\gamma_t)\phi_t + k[\sigma_t^{\phi_t}]\bar{\phi}_t \,, \\ i\partial_t\gamma_t &= \left[h(\gamma_t^{\phi_t}), \gamma_t\right] + k[\sigma_t^{\phi_t}]\sigma_t^* - \sigma_t k[\sigma_t^{\phi_t}]^* \,, \\ i\partial_t\sigma_t &= \left[h(\gamma_t^{\phi_t}), \sigma_t\right]_+ + \left[k(\sigma_t^{\phi_t}), \gamma_t\right]_+ + k[\sigma_t^{\phi_t}] \,, \end{aligned}$$

where $k(\sigma) := v\#\sigma$, $\gamma^\phi := \gamma + |\phi\rangle\langle\phi|$, and $\sigma^\phi := \sigma + |\phi\rangle\langle\bar{\phi}|$.

If we put $\Gamma_t := \begin{pmatrix} \gamma_t & \sigma_t \\ \bar{\sigma}_t & 1+\bar{\gamma}_t \end{pmatrix}$ and $\hat{\phi}_t := \begin{pmatrix} \phi \\ \bar{\phi}_t \end{pmatrix}$ then the HFB equation is, yet, equivalent to the system

$$i\partial_t \hat{\phi}_t(x) = S\left(\hat{h} + [\hat{v} * \Gamma^{\hat{\phi}_t}]\right) \hat{\phi}_t(x) + \int S\,[\hat{v} \# \Gamma^{\hat{\phi}_t}]\, \phi_t(y)\, dy \; ,$$

$$i\partial_t \Gamma_t = \Gamma_t\big(\hat{h} + [\hat{v} * \Gamma^{\hat{\phi}_t}]\big) S - S\big(\hat{h} + [\hat{v} * \Gamma^{\hat{\phi}_t}]\big)\Gamma_t + \int S\,[\hat{v} \# \Gamma^{\hat{\phi}_t}]\,\Gamma_t - \int \Gamma_t\,[\hat{v} \# \Gamma^{\hat{\phi}_t}]\, S \; ,$$

where $S := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is the natural symplectic form in this framework.

- HF approximation: Hartree, Fock, Slater, Lieb-Simon 1978; time-dependent: Chadam 1976, Zagatti 1992;
- Quasifree states and reduced one-particle density matrices: Robinson 1965, Shale-Stinespring 1965, Araki-Shiraishi 1971, Bach-Lieb-Solovej 1994, Solovej 2007/2014, Bach-Breteaux-Knörr-Menge 2014;
- MF and GP Limit (only γ, no ϕ or σ): Hepp 1974, Ginibre-Velo 1979, Fröhlich-Tsai-Yau 2000, Bardos-Golse-Gottlieb-Mauser 2000-04, Erdős-Schlein-Yau 2007-09, Ammari-Nier 2008-11, Fröhlich-Knowles-Pizzo 2007-11, Grillakis-Machedon 2010-13;

- Approximation of full dynamics by HFB dynamics for fermions: Gottlieb-Mauser 2007, Pickl 2011, Petrat 2015, Benedikter-Porta-Schlein 2014-16, Bach-Breteaux-Petrat-Pickl-Tzaneteas 2016, Porta-Rademacher-Saffirio-Schlein 2017;
- Approximation of full dynamics by MF dynamics for bosons: Erdős-Schlein-Yau 2007-13, Rodnianski-Schlein 2009, Grillakis-Machedon 2010-13;
- Studying (nonlinear) HFB dynamics for fermions: Benedikter-Sok-Solovej 2017;
- Studying (nonlinear) HFB dynamics for bosons (with ϕ, γ, and σ): Grillakis-Machedon 2017, BBCFS 2018;

We introduce suitable Sobolev spaces $(X_j, \| \cdot \|_{X_j})$, with $\big\|(\phi, \gamma, \sigma)\big\|_{X_j} := \|\phi\|_{j,\phi} + \|\gamma\|_{j,\gamma} + \|\sigma\|_{j,\sigma}$ and $\|\phi\|_{j,\phi} := \|M^j \phi\|_{\mathfrak{h}}$, $\|\gamma\|_{j,\gamma} := \|M^j \gamma M^j\|_{\mathcal{L}^1(\mathfrak{h})}$, $\|\sigma\|_{j,\sigma} := \|M^j \sigma\|_{\mathcal{L}^2(\mathfrak{h})} + \|\sigma M^j\|_{\mathcal{L}^2(\mathfrak{h})}$, where $M := \sqrt{1 - \Delta}$.

Thm 1: Assume (H) and that $t \mapsto (\phi_t, \gamma_t, \sigma_t) \in C^1(\mathbb{R}_0^+; X_0) \cap C^1(\mathbb{R}_0^+; X_0)$ is a solution of the HFB equations and ω_t^q is the unique corresponding quasifree state. Then

(A) The particle number is conserved, i.e., for all $t > 0$
$$\mathrm{Tr}(\gamma_t) + \|\phi_t\|_{\mathfrak{h}}^2 = \omega_t^q(\mathbb{N}) = \omega_0^q(\mathbb{N}) = \mathrm{Tr}(\gamma_0) + \|\phi_0\|_{\mathfrak{h}}^2,$$
where $\mathbb{N} = \int \psi^*(x)\psi(x)\, dx$ is the number operator.

(A') More generally, any observable $\mathbb{A}$, which is linear or quadratic in creation and annihilation operators and commutes with $\mathbb{H}$, is conserved, i.e., for all $t > 0$,
$$\omega_t^q(\mathbb{A}) = \omega_0^q(\mathbb{A}).$$

(B) The energy
$\mathcal{E}(\phi_t, \gamma_t, \sigma_t) = \omega_t^q(\mathbb{H}) = \mathrm{Tr}\left\{h\gamma_t^{\phi_t} + b[|\phi\rangle\langle\phi|]\gamma + \frac{1}{2}b[\gamma]\gamma\right\}$
is conserved, i.e., for all $t > 0$

$$\omega_t^q(\mathbb{H}) = \omega_0^q(\mathbb{H}).$$

(C) If $\Gamma_0 := \begin{pmatrix} \gamma_0 & \sigma_0 \\ \bar{\sigma}_0 & 1+\bar{\gamma}_0 \end{pmatrix} \geq 0$ then $\Gamma_t := \begin{pmatrix} \gamma_t & \sigma_t \\ \bar{\sigma}_t & 1+\bar{\gamma}_t \end{pmatrix} \geq 0$, for all $t > 0$.

Thm 2: Assume (H') and that $(\phi_0, \gamma_0, \sigma_0) \in X_1$. Then the HFB equations possesses a unique global solution

$$t \mapsto (\phi_t, \gamma_t, \sigma_t) \in C^1(\mathbb{R}_0^+; X_0) \cap C^1(\mathbb{R}_0^+; X_0).$$

Thm 3: Construction of Gibbs States and condensate for $\beta < \infty$.