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PhD thesis

One Dimensional Dilute Quantum Gases and Their Ground State Energies

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Many-Body Quantum Mechanics

In this chapter we give a brief introduction to many-body quantum mechanics. The chapter will serve to define relevant quantities, to set up the mathematical framework, and to state some preliminary results.

Many-body Wave Functions

In quantum mechanics a system is described by a *state* or *wave function* in an underlying Hilbert space.

Definition 1. *A quantum system at fixed time is a pair*

$$(\Psi, \mathcal{H}), \text{ with } \Psi \in \mathcal{H} \text{ and } \|\Psi\| = 1,$$

where $\mathcal{H}$ is a Hilbert space. Here Ψ is called the state or wave function of the system.

In this thesis, we are mostly interested in quantum system consisting of N particles in a region $\Omega \subseteq \mathbb{R}^d$, possibly with spin degrees of freedom $\{S_i\}_{i\in 1,\dots,N}$. We refer to d as the *dimension* of the system. Such a system is described by having

$$\mathcal{H} = L^2\left(\prod_{i=1}^{N} (\Omega \times \{-S_i, ..., S_i\})\right) = \otimes_{i=1}^{N} L^2\left(\Omega; \mathbb{C}^{2S_i+1}\right),$$

where S_i is the *spin* of the ith particle. Since we are more specificically interested in identical particles we will further restrict the structure of the underlying Hilbert space below.

Identical Particles: Bosons and Fermions

In the case when the particles in question are identical, *i.e.* indistinguishable, it turn out that one can restrict the underlying Hilbert space, to have certain symmetries. Considering N indistiguishable particles, we restrict to the physical configuration space to $C_{p,N} = C_N/S_N$, with $C_N := \{(x_1, \dots, x_N) \in \Omega^N | x_i \neq x_j \text{ if } i \neq j\}$ on which the symmetric group act freely. For $d \geq 2$, we then require the wave function of the system to take values in a unitary irreducible representation of the fundamental group $\pi_1(C_{p,N})$, where we noted that the physical configuration space is path-connected.

Remark 2. *For $d \geq 3$ we have $\pi_1(C_{p,N}) = S_N$, for $d = 2$ we have $\pi_1(C_{p,N}) = B_N$ and for $d = 1$ we have $\pi_1(C_{p,N}) = \{1\}$. In the somewhat special case of $d = 1$, $C_{p,N} = \{x_1 < x_2 < \ldots < x_N\}$. On this configuration space one can never interchange particles without crossing the singular excluded incidence (hyper)planes. Thus the allowed particle statistics are determined by the possible permutation invariant dynamics (see section below) on this space. In section ... we will see examples of different particle statistics in one dimension.*

Remark 3. *Adding spin to the above considerations amounts to having $C_N := \{(z_1, \dots, z_N) \in (\Omega \times \{-S, \dots, S\})^N | (z_i)_1 \neq (z_j)_1 \text{ if } i \neq j\}$, and $C_{p,N} := C_N/S_N$. In this case $C_{p,N}$ is not path connected, however, for each configuration of spins $\sigma = (\sigma_1, \dots, \sigma_N) \in \{-S, \dots, S\}^N$ the configurations spaces $C_{p,N,\sigma} = \{((x_1, \sigma_1), \dots, (x_N, \sigma_N)) \in (\Omega \times \{-S, \dots, S\})^N | x_i \neq x_j \text{ if } i \neq j\}$ are path connected and their fundamental groups are isomorphic to the fundamental group in the spinless case indepent of σ.*
Alternatively, one can view the wave function as a $(2S+1)^N$-dimensional vector bundle over the physical (spinless) configuration space.

In the remaining part of this thesis, we will mainly be interested in the two irreducible representations that are the symmetric representation and the antisymmetric representation, in which we refer to the particles as *bosons* and *fermions* respectively. It is an empiracal fact that bosons and fermions are the only types of elementary particles that are encountered in nature. Hence for bosons we restrict to wave functions in the symmetric (or bosonic) subspace $L^2_s\left((\Omega \times \{-S, \dots, S\})^N\right) \cong \vee_{i=1}^N L^2\left(\Omega; \mathbb{C}^{2S+1}\right)$ and for fermions we restrict to wave-functions in the antisymmetric (or fermionic) subspace $L^2_a\left((\Omega \times \{-S, \dots, S\})^N\right) \cong \wedge_{i=1}^N L^2\left(\Omega; \mathbb{C}^{2S+1}\right)$.
To recap we list the following important definitions

Definition 4. *A quantum system of N spin–S bosons in $\Omega \subseteq \mathbb{R}^d$ at fixed time is a pair*

$$(\Psi, \mathcal{H}), \text{ with } \Psi \in \mathcal{H} \text{ and } \|\Psi\| = 1,$$

where $\mathcal{H} = L^2_s\left((\Omega \times \{-S, \dots, S\})^N\right) \cong \vee_{i=1}^N L^2\left(\Omega; \mathbb{C}^{2S+1}\right)$.

Definition 5. *A quantum system of N spin–S fermions in $\Omega \subseteq \mathbb{R}^d$ at fixed time is a pair*

$$(\Psi, \mathcal{H}), \text{ with } \Psi \in \mathcal{H} \text{ and } \|\Psi\| = 1,$$

where $\mathcal{H} = L^2_a\left((\Omega \times \{-S, \ldots, S\})^N\right) \cong \wedge_{i=1}^N L^2\left(\Omega; \mathbb{C}^{2S+1}\right)$.

Observables, Dynamics, and Energy

In general we call any self-adjoint operator on $\mathcal{H}$ an *observable*. Physically, observables represent quanteties that, in principle, can be measured in an experiment. It is a postulate of quantum mechanics that given an observable $\mathcal{O} = \int_{\sigma(\mathcal{O})} \lambda \, \mathrm{d}P_\lambda$, where $\{P_\lambda\}_{\lambda \in \sigma(\mathcal{O})}$ is the projection valued measure associated to $\mathcal{O}$ by the spectral theorem (ref Reed and Simon.), the probabilty of a measurement of $\mathcal{O}$ in state $\Psi \in \mathcal{D}(\mathcal{O})$ having outcome $\lambda \in M \subset \mathbb{R}$ is given by $P((\mathcal{O}, \Psi) \to \lambda \in M) = \int_{\lambda \in M} \langle \Psi, P_\lambda \Psi \rangle$. Furhtermore we defined the expected value of an observable.

Definition 6. *The expectation value of an observable $\mathcal{O}$ in state $\Psi \in \mathcal{D}(\mathcal{O})$ is*

$$\langle \mathcal{O} \rangle_\Psi := \int_{\lambda \in \sigma(\mathcal{O})} \lambda \, \langle \Psi, P_\lambda \Psi \rangle$$

where $\{P_\lambda\}_{\lambda \in \sigma(\mathcal{O})}$ is the projection valued measure associated to $\mathcal{O}$ by the spectral theorem.

I the previous section we defined a quantum system at a fixed time. However, we are often interested in dynamics of the system. In quantum mechanics, time evolution is modelled by the infinitesimal generator of time evolution, H, also known as the *Hamiltonian*. We will in this thesis take H to be a (time-independent) lower bounded self-adjoint operator on $\mathcal{H}$. A state evolves in time according to the Schrödinger equation

$$\Psi(t) = \exp\left(-iH(t - t_0)\right) \Psi(t_0),$$

where have set $\hbar = 1$.

Remark 7. *By Stone's theorem (ref Reed and Simon), the existance of a self-adjoint Hamiltonian, H, is guaranteed for any time evolutions described by $\Psi(t) = U(t - t_0)\Psi(t_0)$, when $U(t)$ is a strongly continous one-parameter unitary group.*

Since the Hamiltonian, H, is self-adjoint, it represents an obersvable which we call *energy*. Since H is lower bounded, there is a natural notion of lowest energy of H.

Definition 8. *The ground state energy of H is defined by*

$$E_0(H) := \inf(\sigma(H))$$

Furthermore, we define the notion of a *ground state* of H as

Definition 9. *We say that a (normalized) state $\Psi \in \mathcal{D}(H) \subset \mathcal{H}$ is a ground state of H if*

$$\langle H \rangle_\Psi = E_0(H).$$

When studying ground states and ground state energies it is useful to have the following variational characterization.

Remark 10. *It follows from the spectral theorem (ref Reed and Simon) that the ground state energy is given by*

$$E_0(H) = \inf_{\Psi \in \mathcal{D}(\mathcal{H})} \frac{\langle \Psi, H\Psi \rangle}{\|\Psi\|^2}. \tag{2.0.1}$$

Remark 11. *It is straightforward to show that the quadratic form $\mathcal{D}(H) \ni \Psi \mapsto \langle \Psi, H\Psi \rangle$ is lower bounded and closable, since H is lower bounded and self-adjoint.*

Definition 12. *Given a Hamitonian, H, we define the associated energy quadratic form, $\mathcal{E}_H : \mathcal{D}(\mathcal{E}_\mathcal{H}) \to \mathbb{R}$, as the closure of the quadratic form $\mathcal{D}(H) \ni \Psi \mapsto \langle \Psi, H\Psi \rangle$. When H is given from the context, we will often write $\mathcal{E}$ as short for $\mathcal{E}_H$.*

Remark 13. *From the definition of $\mathcal{E}_\mathcal{H}$ and from Remark 10 it follows straigthforwardly that we have*

$$E_0(H) = \inf_{\Psi \in \mathcal{D}(\mathcal{E}_\mathcal{H})} \frac{\mathcal{E}_\mathcal{H}(\Psi)}{|\Psi|^2} = \inf_{\substack{\Psi \in \mathcal{D}(\mathcal{E}_\mathcal{H}), \\ \|\Psi\|=1}} \mathcal{E}_\mathcal{H}(\Psi), \tag{2.0.2}$$

as $\mathcal{D}(H)$ is form core for $\mathcal{E}_\mathcal{H}$.

We refer to both (2.0.1) and (2.0.2) as *the variational principle*. We will often in the remaining take (2.0.2) as the vary definition of the ground state energy. Furthermore, one can also define the dynamics of a quantum system by specifying an energy quadratic form in the following sense

Remark 14 (Ref!!)**.** *Given a closable, lower bounded, quadratic for $\mathcal{E} : \mathcal{D}(\mathcal{E}) \to \mathbb{R}$ there exist a* ***unique*** *lower bounded, self-adjoint operator $H_\mathcal{E}$, such that $\mathcal{E}(\Psi) = \langle \Psi, H_\mathcal{E}\Psi \rangle$ for all $\Psi \in \mathcal{D}(H_\mathcal{E})$, and $\mathcal{D}(H_\mathcal{E})$ is form core for $\overline{\mathcal{E}}$,* i.e. *the form closure of $\langle \cdot, H_\mathcal{E} \cdot \rangle$ is equal to the form closure of $\mathcal{E}$.*

Thus we will frequently change between the two equivalent formulations of the dynamics of a quantum system that are the operator, H, formulation and the quadratic form, $\mathcal{E}$, formulation

Many-Body Hamiltonians

Until this point, we have not specified the class of Hamiltonians that we will be interested in. We have seen, that we will care mainly about Hamiltonians defined on the bosonic or fermionic subspaces, however no specification has been made about the dynamics on these subspaces. We are interested in modeling N particles in some region $\Omega \subseteq \mathbb{R}^d$ that interact locally with each other. In practice, this means that the Hamiltonian *formally* takes the form

$$H = \sum_{i=1}^{N} T_i + U(x_1, \ldots, x_N) \tag{2.0.3}$$

where T_i is the *kinetic energy operator* for particle i and the *potential* U is a multiplication operator which models the local interaction among the particles. The kinetic energy operator is taken to be[1]

$$T_i = -\frac{1}{2m_i}\Delta_i \qquad (\hbar = 1) \tag{2.0.4}$$

since we interested in identical particles, we will from this point onwards choose $m_i = 1/2$. As for the potential, V, we of course immediately restrict to permutation-invariant function, U, for identical particles. However, in the following we will further restrict to a combination of having a trapping potential and radial pair potentials, which model pairwise interactions that only depend on the distances between particles. Such potentials take the form

$$U(x_1, \ldots, x_N) = \sum_{i<j} v(x_i - x_j) + \sum_{i=1}^{N} V(x_i) \tag{2.0.5}$$

where we take v to be a radial function and, V, is called the *trapping potential*. We will generally take v to be repulsive, meaning $v \geq 0$, with compact support This includes the case where v is a measure of compact support. The trapping potential we will disregard *i.e.* $V = 0$.

[1] This is usually justified by going through a canonical quanitzation procedure for the classical Hamiltonian function of the system, we are interedsted in modelling