ON THE MINIMIZATION OF HAMILTONIANS OVER PURE GAUSSIAN STATES

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A Hamiltonian defined as a polynomial in creation and annihilation operators is considered. After a minimization of its expectation value over pure Gaussian states, the Hamiltonian is Wick-ordered in creation and annihilation operators adapted to the minimizing state. It is shown that this procedure eliminates from the Hamiltonian terms of degrees 1 and 2 that do not preserve the particle number, and leaves only the terms that can be interpreted as quasiparticles excitations. We propose to call this fact *Beliaev's Theorem*, since to our knowledge it was mentioned for the first time in a paper by Beliaev from 1959.

1. Introduction

Various phenomena in many-body quantum physics are explained with help of *quasiparticles*. Unfortunately, we are not aware of a rigorous definition of this concept, except for some very special cases.

A typical situation when one speaks about quasiparticles seems to be the following: Suppose that the Hamiltonian of a system can be written as $H = H_0 + V$, where H_0 is in some sense dominant and V is a perturbation that in first approximation can be neglected. Suppose also that

$$H_0 = B + \sum_i \omega_i b_i^* b_i, \tag{1.1}$$

where B is a number, operators b_i^*/b_i satisfy the standard canonical commutation/anticommutation relations (CCR/CAR) and the Hilbert space contains a state annihilated by b_i (the *Fock vacuum for* b_i). We then say that the operators b_i^*/b_i *create/annihilate a quasiparticle*.

Of course, the above definition is very vague.

In our paper we describe a simple theorem that for many Hamiltonians gives a natural decomposition $H = H_0 + V$ with H_0 of the form (1.1), and thus suggests a possible definition of a quasiparticle. Our starting point is a fairly general Hamiltonian H defined on a bosonic or fermionic Fock space. For simplicity we assume that the 1-particle space is finite dimensional. With some technical assumptions, the whole picture should be easy to generalize to the infinite dimensional case. We assume that the Hamiltonian is a polynomial in creation and annihilation operators a_i^*/a_i, $i = 1, \dots, n$. (This is a typical assumption in Many Body Quantum Physics and Quantum Field Theory.)

An important role in Many Body Quantum Physics is played by the so-called *Gaussian states*, called also *quasi-free states*. Gaussian states can be *pure* or *mixed*. The former are typical for the zero temperature, whereas the latter for positive temperatures. In our paper we do not consider mixed Gaussian states.

Pure Gaussian states are obtained by applying Bogoliubov transformations to the Fock vacuum state (given by the vector Ω annihilated by a_i's). Pure Gaussian states are especially convenient for computations.

We minimize the expectation value of the Hamiltonian H with respect to pure Gaussian states, obtaining a state given by a vector $\tilde{\Omega}$. By applying an appropriate Bogoliubov transformation, we can replace the old creation and annihilation operators a_i^*, a_i by new ones b_i^*, b_i, which are adapted to the "new vacuum" $\tilde{\Omega}$, i.e., that satisfy $b_i\tilde{\Omega} = 0$. We can rewrite the Hamiltonian H in the new operators and Wick order them, that is, put b_i^* on the left and b_i on the right. The theorem that we prove says that

$$H = B + \sum_{ij} D_{ij} b_i^* b_j + V,$$

where V has only terms of the order greater than 2. In particular, H does not contain terms of the type b_i^*, b_i, $b_i^* b_j^*$, or $b_i b_j$. It is thus natural to set $H_0 := B + \sum_{ij} D_{ij} b_i^* b_j$. D_{ij} is a hermitian matrix. Clearly, it can be diagonalized, so that H_0 acquires the form of (1.1).

We present several versions of this theorem. First we assume that the Hamiltonian is even. In this case it is natural to restrict the minimization to even pure Gaussian states. In the fermionic case, we can also minimize over odd pure Gaussian states. In the bosonic case, we consider also Hamiltonians without the evenness assumption, and then we minimize with respect to all pure Gaussian states.

The procedure of minimizing over Gaussian states is widely applied in practical computations and is known under many names. In the fermionic case in the contex of nuclear physics it often goes under the name of the *Hartree-Fock-Bogoliubov method* [11]. It is closely related to the *Bardeen-Cooper-Schrieffer approximation* used in superconductivity [1] and the *Fermi liquid theory* developed by Landau [10]. In the bosonic case it is closely related to the *Bogoliubov approximation* used in the theory of superfluidity [4], see also [12, 5]. In both bosonic and fermionic cases it is often called the *mean-field approach* [8].

The fact that we describe in our paper is probably very well known, at least on the intuitive level, to many physicists, especially in condensed matter theory. One can probably say that it summarizes in abstract terms one of the most widely used methods of contemporary quantum physics. The earliest reference that we know to a statement similar to our main result is formulated in a paper of Beliaev [2]. Beliaev studied fairly general fermionic Hamiltonians by what we would nowadays call the Hartree-Fock-Bogoliubov approximation. In a footnote on page 10 he writes:

The condition $H_{20} = 0$ may be easily shown to be exactly equivalent to the requirement of a minimum "vacuum" energy U. Therefore, the ground state of the system in terms of new particles is a "vacuum" state. The excited states are characterized by definite numbers of new particles, elementary excitations.

Therefore, we propose to call the main result of our paper *Beliaev's Theorem.*

The proof of Beliaev's Theorem is not difficult, especially when it is formulated in an abstract way, as we do. Nevertheless, in concrete situations, when similar computations are performed, consequences of this result may often appear somewhat miraculous. The authors of this work witnessed it several times: the authors themselves, or their colleagues, after tedious computations and numerous mistakes watched the unwanted terms disappear [5, 6]. As we show, these terms have to disappear by a general argument.

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2. Preliminaries

2.1. *2nd quantization*

We will consider in parallel the bosonic and fermionic case.

Let us describe our notation concerning the 2nd quantization. We will always assume that the 1-particle space is $\mathbb{C}^n$. (It is easy to extend our analysis to the infinite dimensional case.) The *bosonic Fock space* will be denoted $\Gamma_{\mathrm{s}}(\mathbb{C}^n)$ and the *fermionic Fock space* $\Gamma_{\mathrm{a}}(\mathbb{C}^n)$. We use the notation $\Gamma_{\mathrm{s/a}}(\mathbb{C}^n)$ for either the bosonic or fermionic Fock space. $\Omega \in \Gamma_{\mathrm{s/a}}(\mathbb{C}^n)$ stands for the *Fock vacuum.* If r is an operator on $\mathbb{C}^n$, then $\Gamma(r)$ stands for its *2nd quantization*, that is

$$\Gamma(r) := \left(\mathop{\oplus}_{n=0}^{\infty} r^{\otimes n} \right) \Big|_{\Gamma_{\mathrm{s/a}}(\mathbb{C}^n)}.$$

a_i^*, a_i denote the standard *creation* and *annihilation operators* on $\Gamma_{\mathrm{s/a}}(\mathbb{C}^n)$, satisfying the usual canonical commutation/anticommutation relations.

2.2. *Wick quantization*

Consider an arbitrary polynomial on $\mathbb{C}^n$, that is a function of the form

$$h(\overline{z}, z) := \sum_{\alpha,\beta} h_{\alpha,\beta} \overline{z}^{\alpha} z^{\beta}, \tag{2.1}$$

where $z = (z_1, \ldots, z_n) \in \mathbb{C}^n$, $\overline{z}$ denotes the complex conjugate of z and $\alpha = (\alpha_1, \ldots, \alpha_n) \in (\mathbb{N} \cup \{0\})^n$ represent multiindices. In the bosonic/fermionic case we always assume that the coefficients $h_{\alpha,\beta}$ are symmetric/antisymmetric separately in the indices of $\overline{z}$ and z.

We write $|\alpha| = \alpha_1 + \cdots + \alpha_n$. We say that h is *even* if the sum in (2.1) is restricted to even $|\alpha| + |\beta|$.

The Wick quantization of (2.1) is the operator on $\Gamma_{\mathrm{s/a}}(\mathbb{C}^n)$ defined as

$$h(a^*, a) := \sum_{\alpha,\beta} h_{\alpha,\beta}(a^*)^\alpha a^\beta. \tag{2.2}$$

In the fermionic case, (2.2) defines a bounded operator on $\Gamma_{\mathrm{a}}(\mathbb{C}^n)$. In the bosonic case, (2.2) can be viewed as an operator on $\bigcap_{n>0} \mathrm{Dom} N^n \subset \Gamma_{\mathrm{s}}(\mathbb{C}^n)$, where

$$N = \sum_{i=1}^{n} a_i^* a_i$$

is the number operator.

2.3. *Bogoliubov transformations*

We will now present some basic well known facts about Bogoliubov transformations. For proofs and additional information we refer to [3] (see also [7], [9]). We will often use the summation convention of summing with respect to repeated indices.

Operators of the form

$$Q = \theta_{ij} a_i^* a_j^* + h_{kl} a_k^* a_l + \overline{\theta}_{ij} a_j a_i \pm \frac{1}{2} h_{kk}, \tag{2.3}$$

where h is a self-adjoint matrix, will be called *quadratic Hamiltonians*. In the bosonic/fermionic case we can always assume that θ is symmetric/antisymmetric. (The term $\pm\frac{1}{2}h_{kk}$, with the sign depending on the bosonic/fermionic case, means that Q is the Weyl quantization of the corresponding quadratic expression.) The group generated by operators of the form $\mathrm{e}^{\mathrm{i}Q}$, where Q is a quadratic Hamiltonian, is called the *metaplectic (Mp)* group in the bosonic case and the *Spin* group in the fermionic case.

In the bosonic case, the group generated by Mp together with $\mathrm{e}^{\mathrm{i}(y_i a_i^* + \overline{y}_i a_i)}$, $y_i \in \mathbb{C}$, $i = 1, \ldots, n$, is called the *affine mataplectic (AMp)* group.

In the fermionic case, the group generated by operators $y_i a_i^* + \overline{y}_i a_i$ with $\sum |y_i|^2 = 1$ (which are unitary) is called the *Pin* group. Note that *Spin* is a subgroup of *Pin* of index 2.

In the bosonic case, consider $U \in AMp$. It is well known that

$$Ua_iU^* = p_{ij}a_j + q_{ij}a_j^* + \xi_i, \quad Ua_i^*U^* = \overline{p}_{ij}a_j^* + \overline{q}_{ij}a_j + \overline{\xi}_i \tag{2.4}$$

for some matrices p and q and a vector ξ.

In the fermionic case, consider $U \in Pin$. Then

$$Ua_iU^* = p_{ij}a_j + q_{ij}a_j^*, \quad Ua_i^*U^* = \overline{p}_{ij}a_j^* + \overline{q}_{ij}a_j \tag{2.5}$$

for some matrices p and q.

The maps (2.4) and (2.5) are often called *Bogoliubov transformations*. Bogoliubov transformations can be interpreted as automorphism of the corresponding *classical phase space*. Let us describe briefly this interpretation.

Consider the space $\mathbb{C}^n \oplus \mathbb{C}^n$. It has a distinguished $2n$-dimensional real subspace consisting of vectors $(z, \overline{z}) = ((z_i)_{i=1,\dots,n}, (\overline{z}_i)_{i=1,\dots,n})$, which we will call *the real part of* $\mathbb{C}^n \oplus \mathbb{C}^n$, and which can be interpreted as the classical phase space. The real part of $\mathbb{C}^n \oplus \mathbb{C}^n$ is equipped with a symplectic form

$$(z, \overline{z})\omega(z', \overline{z}') := \mathrm{Im}(z|z'), \tag{2.6}$$

and a scalar product

$$(z, \overline{z}) \cdot (z', \overline{z}') := \mathrm{Re}(z|z'). \tag{2.7}$$

Consider the bosonic case. Note that the transformation (2.4), viewed as a map on the real part of $\mathbb{C}^n \oplus \mathbb{C}^n$ given by the matrix $\begin{bmatrix} p & q \\ \overline{q} & \overline{p} \end{bmatrix}$ and the vector $\begin{bmatrix} \xi \\ \overline{\xi} \end{bmatrix}$, preserves the symplectic form (2.6) – in other words, it belongs to ASp, the *affine symplectic group*. More precisely, it is easily checked that in this way we obtain a 2-fold covering homomorphism of AMp onto ASp.

In the fermionic case there is an analogous situation. The transformation (2.5), viewed as a map on the real part of $\mathbb{C}^n \oplus \mathbb{C}^n$ given by the matrix $\begin{bmatrix} p & q \\ \overline{q} & \overline{p} \end{bmatrix}$, preserves the scalar product (2.7) – in other words, it belongs to O, the *orthogonal group*. More precisely, it is easily checked that in this way we obtain a 2-fold covering homomorphism of Pin onto O.

2.4. *Pure Gaussian states*

We will use the term *pure state* to denote a normalized vector modulo a phase factor. In particular, we will distinguish between a pure state and its *vector representative*.

On Fock spaces we have a distinguished pure state called the *(Fock) vacuum state*, corresponding to Ω. States given by vectors of the form $U\Omega$, where $U \in Mp$ or $U \in Spin$, will be called *even pure Gaussian states.* The family of even pure Gaussian states will be denoted by $\mathfrak{G}_{\mathrm{s/a},0}$.

In the bosonic case, states given by vectors of the form $U\Omega$ where $U \in AMp$ will be called *Gaussian pure states.* The family of bosonic pure Gaussian states will be denoted by $\mathfrak{G}_{\mathrm{s}}$.

In the fermionic case, states given by vectors of the form $U\Omega$, where $U \in Pin$ will be called *fermionic pure Gaussian states.* The family of fermionic pure Gaussian states is denoted $\mathfrak{G}_{\mathrm{a}}$.

Fermionic pure Gaussian states that are not even will be called *odd fermionic pure Gaussian states.* The family of odd fermionic pure Gaussian states is denoted $\mathfrak{G}_{\mathrm{a},1}$.

One can ask whether pure Gaussian states have *natural* vector representatives (that is, whether one can naturally fix the phase factor of their vector representatives). In the bosonic case this is indeed always possible. If $c = [c_{ij}]$ is a symmetric matrix satisfying $\|c\| < 1$, then the vector

$$\det(1 - c^*c)^{1/4} \mathrm{e}^{\frac{1}{2} c_{ij} a_i^* a_j^*} \Omega \tag{2.8}$$

defines a state in $\mathfrak{G}_{\mathrm{s},0}$ (see [13]). If $\theta = [\theta_{ij}]$ is a symmetric matrix satisfying $c = \mathrm{i}\frac{\tanh\sqrt{\theta\theta^*}}{\sqrt{\theta\theta^*}}\theta$, then (2.8) equals

$$\mathrm{e}^{\mathrm{i}X_\theta}\Omega \tag{2.9}$$

with

$$X_\theta := \theta_{ij} a_i^* a_j^* + \overline{\theta}_{ij} a_j a_i. \tag{2.10}$$

Each state in $\mathfrak{G}_{\mathrm{s},0}$ is represented uniquely as (2.8) (or equivalently as (2.9)). In particular, (2.9) provides a smooth parametrization of $\mathfrak{G}_{\mathrm{s},0}$ by symmetric matrices.

The manifold of fermionic even pure Gaussian states is more complicated. We will say that a fermionic even pure Gaussian state given by Ψ is *nondegenerate* if $(\Omega|\Psi) \neq 0$ (if it has a nonzero overlap with the vacuum). Every nondegenerate fermionic even pure Gaussian state can be represented by a vector

$$\det(1 + c^*c)^{-1/4} \mathrm{e}^{\frac{1}{2} c_{ij} a_i^* a_j^*} \Omega, \tag{2.11}$$

where $c = [c_{ij}]$ is an antisymmetric matrix. If $\theta = [\theta_{ij}]$ is an antisymmetric matrix satisfying $c = \mathrm{i}\frac{\tan\sqrt{\theta\theta^*}}{\sqrt{\theta\theta^*}}\theta$, $\|\theta\| < \pi/2$, then (2.11) equals

$$\mathrm{e}^{\mathrm{i}X_\theta}\Omega \tag{2.12}$$

with

$$X_\theta := \theta_{ij} a_i^* a_j^* + \overline{\theta}_{ij} a_j a_i. \tag{2.13}$$

Vectors (2.11) are natural representatives of their states. It is easy to see that only nondegenerate fermionic pure Gaussian states possess natural vector representatives.

Not all even fermionic pure Gaussian states are nondegenerate. *Slater determinants* with an even nonzero number of particles are examples of even Gaussian pure states that are not nondegenerate.

Nondegenerate pure Gaussian states form an open dense subset of $\mathfrak{G}_{\mathrm{a},0}$ containing the Fock state (corresponding to $c = \theta = 0$). In particular, (2.11) provides a smooth parametrization of a neighborhood of the Fock state in $\mathfrak{G}_{\mathrm{a},0}$ by antisymmetric matrices.

The fact that each even bosonic/nondegenerate fermionic pure Gaussian state can be represented by a vector of the form (2.8)/(2.11) goes under the name of the *Thouless Theorem*. (See [14]; this name is used eg. in the monograph by Ring and Schuck [11].) The closely related fact saying that these vectors can be represented in the form (2.9)/(2.12) is sometimes called the *Ring-Schuck Theorem.*

By definition, the group AMp/Pin acts transitively on $\mathfrak{G}_{\mathrm{s/a}}$. In other words, for any $\tilde{\Omega} \in \mathfrak{G}_{\mathrm{s/a}}$ we can find $U \in AMp/Pin$ such that $\tilde{\Omega} = U\Omega$. Such a U is not defined uniquely – it can be replaced by $U\Gamma(r)$, where r is unitary on $\mathbb{C}^n$.

Clearly, if we set

$$b_i := U a_i U^*, \quad b_i^* := U a_i^* U^*, \tag{2.14}$$

then $b_i\tilde{\Omega} = 0$, $i = 1, \ldots, n$, and they satisfy the same CCR/CAR as a_i, $i = 1, \ldots, n$. If h is a polynomial of the form (2.1), then we can Wick quantize it using the transformed operators:

$$h(b^*, b) = \sum_{\alpha,\beta} h_{\alpha,\beta} (b^*)^\alpha b^\beta.$$

Obviously, $Uh(a^*, a)U^* = h(b^*, b)$.

3. Main Result

As explained in the introduction, we think that the following result should be called *Beliaev's Theorem.*

Theorem 3.1: *Let h be a polynomial on $\mathbb{C}^n$ and $H := h(a^*, a)$ its Wick quantization. We consider the following functions:*

(1) *(bosonic case, even pure Gaussian states)* $\mathfrak{G}_{\mathrm{s},0} \ni \Phi \mapsto (\Phi|H\Phi)$;
(2) *(bosonic case, arbitrary pure Gaussian states)* $\mathfrak{G}_{\mathrm{s}} \ni \Phi \mapsto (\Phi|H\Phi)$;
(3) *(fermionic case, even pure Gaussian states)* $\mathfrak{G}_{\mathrm{a},0} \ni \Phi \mapsto (\Phi|H\Phi)$;
(4) *(fermionic case, odd pure Gaussian states)* $\mathfrak{G}_{\mathrm{a},1} \ni \Phi \mapsto (\Phi|H\Phi)$.

In (1), (3) and (4) we assume in addition that the polynomial h is even.

For a vector $\tilde{\Omega}$ representing a pure Gaussian state, let $U \in AMp/Pin$ satisfy $\tilde{\Omega} = U\Omega$. Set $b_i = Ua_iU^*$ and suppose that $\tilde{h}$ is the polynomial satisfying $H = \tilde{h}(b^*, b)$. Then the following statements are equivalent:

(A) $\tilde{\Omega}$ represents a stationary point of the function defined in (1)–(4).

(B)

$$\tilde{h}(b^*, b) = B + D_{ij}b_i^*b_j + \text{terms of higher order in } b\text{'s}.$$

Proof: Let us prove the case (2), which is a little more complicated than the remaining cases. Let us fix $U \in AMp$ so that $\tilde{\Omega} = U\Omega$. Clearly, we can write

$$H = \tilde{h}(b^*, b) = B + \overline{K}_ib_i + K_ib_i^* + O_{ij}b_j^*b_i^* + \overline{O}_{ij}b_ib_j + D_{ij}b_i^*b_j \\ + \text{terms of higher order in } b\text{'s}. \tag{3.1}$$

We know that in a neighborhood of $\tilde{\Omega}$ arbitrary pure Gaussian states are parametrized by a symmetric matrix θ and a vector y:

$$\theta \mapsto U\mathrm{e}^{\mathrm{i}\phi(y)}\mathrm{e}^{\mathrm{i}X_\theta}\Omega,$$

where $X_\theta := \theta_{ij}a_i^*a_j^* + \overline{\theta}_{ij}a_ja_i$ and $\phi(y) = y_ia_i^* + \overline{y}_ia_i$. We get

$$(U\mathrm{e}^{\mathrm{i}\phi(y)}\mathrm{e}^{\mathrm{i}X_\theta}\Omega|HU\mathrm{e}^{\mathrm{i}\phi(y)}\mathrm{e}^{\mathrm{i}X_\theta}\Omega) = (\mathrm{e}^{\mathrm{i}\phi(y)}\mathrm{e}^{\mathrm{i}X_\theta}\Omega|U^*\tilde{h}(b^*, b)U\mathrm{e}^{\mathrm{i}\phi(y)}\mathrm{e}^{\mathrm{i}X_\theta}\Omega) \\ = (\Omega|\mathrm{e}^{-\mathrm{i}X_\theta}\mathrm{e}^{-\mathrm{i}\phi(y)}\tilde{h}(a^*, a)\mathrm{e}^{\mathrm{i}\phi(y)}\mathrm{e}^{\mathrm{i}X_\theta}\Omega). \tag{3.2}$$

Now

$$\mathrm{e}^{-\mathrm{i}X_\theta}\mathrm{e}^{-\mathrm{i}\phi(y)}\tilde{h}(a^*, a)\mathrm{e}^{\mathrm{i}\phi(y)}\mathrm{e}^{\mathrm{i}X_\theta} = B - \mathrm{i}(\overline{\theta}_{ij}O_{ij} - \theta_{ij}\overline{O}_{ij}) - \mathrm{i}(\overline{y}_iK_i - y_i\overline{K}_i) \\ + \text{terms containing } a_i \text{ or } a_i^* \; + O(\|\theta\|^2, \|y\|^2).$$

Therefore, (3.2) equals

$$B - \mathrm{i}(\overline{\theta}_{ij}O_{ij} - \theta_{ij}\overline{O}_{ij}) - \mathrm{i}(\overline{y}_iK_i - y_i\overline{K}_i) + O(\|\theta\|^2, \|y\|^2). \tag{3.3}$$

Since vectors y and matrices θ are independent variables, (3.3) is stationary at $\tilde{\Omega}$ if and only if $[O_{ij}]$ is a zero matrix and $[K_i]$ is a zero vector. This ends the proof of part (2).

To prove (3) and (4) we note that, for $U \in Pin$, the neighborhood of $\tilde{\Omega} = U\Omega$ in the set of fermionic pure Gaussian states is parametrized by antisymmetric matrices θ:

$$\theta \mapsto U\mathrm{e}^{iX_\theta}\Omega,$$

where again $X_\theta := \theta_{ij}a_i^* a_j^* + \overline{\theta}_{ij}a_j a_i$. Therefore, it suffices to repeat the above proof with $y_i = K_i = 0$, $i = 1, \ldots, n$.

The proof of (1) is similar. □

Proposition 3.2: *In addition to the assumptions of Theorem 3.1 (2), suppose that $\tilde{\Omega}$ corresponds to a minimum. Then the matrix $[D_{ij}]$ is positive.*

Proof: Using that O and K are zero, we obtain

$$\mathrm{e}^{-\mathrm{i}\phi(y)}\tilde{h}(a^*, a)\mathrm{e}^{\mathrm{i}\phi(y)} = B + \overline{y}_i D_{ij} y_j + \text{terms containing } a_i \text{ or } a_i^* \ + O(\|y\|^3).$$

Therefore, (3.2) equals

$$B + \overline{y}_i D_{ij} y_j + O(\|y\|^3). \tag{3.4}$$

Hence the matrix $[D_{ij}]$ is positive. □

Note that in cases (1), (3) and (4) the matrix $[D_{ij}]$ does not have to be positive.

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