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Symmetry Breaking for a Non-linear Schrödinger Equation

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Abstract. We define a notion of stability for molecular states and show that the stable ground states of a molecular Hamiltonian are not unique (break rotational symmetry) if the atomic masses are greater than certain finite critical values. The stable ground states are stationary with respect to a new non-linear Schrödinger equation, which is exactly soluble in certain simple cases.

§ 1. Introduction

There has been some interest recently [2, 12, 13] in the problem of the quantum-mechanical justification of the concept of molecular structure. The problem is to explain why it is that in most situations, excluding possibly those of extreme isolation, the wave function of a molecule seems to be not an eigenstate of the Hamiltonian, but one of a class of slowly time varying states which are more stable in some sense.

In this paper we propose a precise definition of stability and prove the existence of stable ground states (Sect. 2). In Sect. 3 we show that for large enough atomic masses and typical two-body interactions the stable ground states are not unique. The breaking of the rotational symmetry of the Hamiltonian which occurs is closely related to the problem of molecular structure, as was pointed out by Woolley [12]. We study the anharmonic oscillator in some detail and show that reflection symmetry (parity) breaking does not occur for small masses and that there is an associated phase transition for finite values of the various parameters.

Having proved in Sect. 2 that the stable ground states satisfy a certain non-linear Schrödinger equation, we devote Sects. 4 and 5 to an analysis of the associated time-dependent one-body Schrödinger equation. Although non-linear we show that it is exactly soluble even in three space dimensions, and clarify some geometrical properties of the solution related to the Euclidean symmetry of the equation. Finally in Sects. 6 and 7 we sketch two possible approaches to the "derivation" of the non-linear Schrödinger equation, firstly using a second quantised linear Hamiltonian describing the interaction of an atom with an external phonon field, and secondly by reference to a collective model of nuclear structure.

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For the sake of simplicity we confine our exposition to the case of two spin zero atoms interacting in three space dimensions, so that wave functions ψ are unit vectors in $L^2(\mathbb{R}^6)$. Much of our analysis can be carried out for n-body systems but there is much extra complication which we prefer to avoid. We therefore assume that the electronic structure has been eliminated by the Born-Oppenheimer method, so that the atoms interact by an effective potential which is attractive at long range and repulsive at short range (precise conditions are given in the next section).

If $\{Q_i\}_{i=1}^6$ are the position operators on $\mathscr{H}$, three for each particle, and ϱ is a density matrix on $\mathscr{H}$, we define

$$W(\varrho) = \sum_{i=1}^{6} \{\mathrm{tr}[Q_i^2 \varrho] - \mathrm{tr}[Q_i \varrho]^2\}$$

and for $\alpha > 0$ minimise

$$\mathrm{tr}[H\varrho] + \alpha W(\varrho)$$

over the set X of all normalised density matrices. The weight $W(\varrho)$ may be interpreted either as the energy of polarisation of the medium in which the atoms travel, or as a measure of the stability of the state ϱ of the atoms. From its form we see that $W(\varrho)$ is unchanged by translation or rotation but decreases as the distribution of the state in position space becomes more concentrated. The single undetermined parameter $\alpha > 0$ measures the total influence of the surrounding medium and presumably increases with its density. In the extreme low density regime we may put $\alpha = 0$ and recover thee usual quantum mechanical theory. These are precisely the circumstances where the justification for the molecular structure hypothesis is least clear [13].

We point out that the above procedure is entirely analogous to one of the derivations of Gibbs states. Namely

$$\varrho_\beta = e^{-\beta H}/\mathrm{tr}[e^{-\beta H}]$$

may be characterized as the density matrix which minimises

$$\mathrm{tr}[H\varrho] + \beta^{-1}\,\mathrm{tr}[\varrho \log \varrho]$$

the second term again being non-linear and representing an influence of the surrounding medium.

From this point onwards however the two discussions proceed along entirely different lines, for $W(\varrho)$ is a concave function on the convex set X. This implies that if the functional does take a minimum value then it takes that value on the pure states (extreme points of X). We therefore reformulate the problem as one of minimising

$$\langle H\psi, \psi\rangle + \alpha W(\psi) \tag{1.1}$$

over all ψ with $\|\psi\| = 1$, where $\alpha > 0$ and

$$W(\psi) = \sum_{i=1}^{6} \{\langle Q_i^2 \psi, \psi\rangle - \langle Q_i \psi, \psi\rangle^2\}. \tag{1.2}$$

§ 2. Existence of the Minimum

We assume that the Hamiltonian H on $\mathscr{H} = L^2(\mathbb{R}^6)$ is of the form

$$H = -\frac{1}{2m_1}\Delta_1 - \frac{1}{2m_2}\Delta_2 + V(x_1 - x_2)$$

where $x_1, x_2 \in \mathbb{R}^3$ are the coordinates of the two particles and V is a pair potential bounded from below. We also assume that V is continuous and central, although this is not needed for several of the theorems. The Hamiltonian is defined as a quadratic form sum and is invariant under the Euclidean group.

We define the domain of the weight W to be

$$\mathrm{Dom}(W) = \bigcap_{i=1}^{6} \mathrm{Dom}(Q_i)$$

on which it is non-negative. We wish to minimise

$$\langle H\psi, \psi\rangle + \alpha W(\psi)$$

for $\alpha > 0$, where $\|\psi\| = 1$ and

$$\psi \in Q(H) \cap \mathrm{Dom}(W) = \mathrm{Dom}(H + Q^2 + C)^{1/2}$$

for all sufficiently large constants C. Any such minimum is called a stable ground state of the Hamiltonian H.

The following theorem has much in common with results of Lieb and Simon [7, 8] on the existence of Hartree-Fock minima for molecular Hamiltonians.

Theorem 2.1. *A stable ground state exists if*

$$V(x) < \lim_{r \to \infty} V(r) = 0$$

for all $x \in \mathbb{R}^3$.

Proof. Let

$$E = \inf\{\langle H\psi, \psi\rangle + W(\psi) : \|\psi\| = 1\}$$

and let ψ_n be a minimising sequence, so that

$$\langle H\psi_n, \psi_n\rangle + W(\psi_n) \leqq E + 1$$

and

$$\langle H\psi_n, \psi_n\rangle + W(\psi_n) \to E.$$

We further suppose, as we may, that the centre of mass of each wave function is at the origin. If

$$-K = \inf\{V(x) : x \in \mathbb{R}^3\}$$

and

$$H_0 = -\frac{1}{2m_1}\Delta_1 - \frac{1}{2m_2}\Delta_2$$

then

$$\langle H_0\psi_n, \psi_n\rangle + W(\psi_n) \leqq K + E + 1\,. \tag{2.1}$$

The left-hand side of (2.1) is invariant with respect to space translations of each particle separately. Therefore there exist space translations $U(a_n, b_n)$ where $a_n, b_n \in \mathbb{R}^3$ and $m_1 a_n + m_2 b_n = 0$, such that if $\varphi_n = U(a_n, b_n)\psi_n$ then

$$\langle Q_i\varphi_n, \varphi_n\rangle = 0$$

and

$$\left\langle \left(H_0 + \alpha \sum_{i=1}^{6} Q_i^2\right)\varphi_n, \varphi_n \right\rangle \leqq K + E + 1$$

for all i and n. Since $\left(H_0 + \alpha \sum_{i=1}^{6} Q_i^2\right)$ has compact resolvent the set

$$\left\{\varphi : \left\langle \left(H_0 + \alpha \sum_{i=1}^{6} Q_i^2\right)\varphi, \varphi \right\rangle \leqq K + E + 1\right\}$$

is norm compact and there is a subsequence, which we still denote by φ_n, such that

$$\lim_{n\to\infty} \|\varphi_n - \varphi\| = 0\,.$$

Moreover

$$\langle Q_i\varphi, \varphi\rangle = \lim_{n\to\infty} \langle Q_i\varphi_n, \varphi_n\rangle = 0$$

for all i, by the convergence of the φ_n, and the uniform boundedness of $\langle Q_i^2\varphi_n, \varphi_n\rangle$.

If we can show that $c_n = (b_n - a_n)$ is bounded then we can pass to another subsequence and assume

$$\lim_{n\to\infty} a_n = a\,; \qquad \lim_{n\to\infty} b_n = b\,.$$

Defining

$$\psi = U(a, b)^*\varphi$$

we see that

$$\lim_{n\to\infty} \psi_n = \psi\,; \qquad \lim_{n\to\infty} \langle Q_i\psi_n, \psi_n\rangle = \langle Q_i\psi, \psi\rangle\,.$$

But

$$\left\langle \left(H_0 + V + \alpha \sum_{i=1}^{6} Q_i^2\right)\psi, \psi \right\rangle \leqq \lim_{n\to\infty} \left\langle \left(H_0 + V + \alpha \sum_{i=1}^{6} Q_i^2\right)\psi_n, \psi_n \right\rangle$$

by the lower semicontinuity of the quadratic form of any semi-bounded self-adjoint operator. Therefore

$$\begin{aligned} &\langle H\psi, \psi\rangle + W(\psi) \\ &\quad = \langle (H_0 + V + \alpha \textstyle\sum Q_i^2)\psi, \psi\rangle - \alpha \sum \langle Q_i\psi, \psi\rangle^2 \\ &\quad \leqq \lim_{n\to\infty} \{\langle H\psi_n, \psi_n\rangle + W(\psi_n)\} = E\,. \end{aligned}$$

To prove that the sequence c_n is bounded we use the equality

$$\langle H\psi_n, \psi_n\rangle + W(\psi_n) = \left\langle \left(H_0 + \alpha \sum_{i=1} Q_i^2\right)\varphi_n, \varphi_n \right\rangle + I_n \tag{2.2}$$

where

$$I_n = \iint V(x-y-c_n)|\varphi_n(x,y)|^2 d^3x d^3y\,. \tag{2.3}$$

Now $\iint (1+x^2+y^2)|\varphi_n(x,y)|^2 d^3x d^3y$

$$\leqq 1 + \alpha^{-1}\langle (H_0 + \alpha \sum Q_i^2)\varphi_n, \varphi_n\rangle$$

$$\leqq 1 + \alpha^{-1}(K+E+1)\,.$$

This implies that there is a constant B such that

$$\iint\limits_{x^2+y^2 \leqq B^2} |\varphi_n(x,y)|^2 d^3x d^3y \geqq \tfrac{1}{2}\,.$$

Now define

$$\max\{V(x-y) : x^2+y^2 \leqq 4B^2\} = -D$$

so that $D>0$. Then $I_n \leqq -\frac{1}{2}D$ if $|c_n| \leqq B$ while

$$I_n \geqq \{1+\alpha^{-1}(K+E+1)\} \min_{x,y} \{(1+x^2+y^2)^{-1} V(x-y-c_n)\}$$

$$\geqq -\tfrac{1}{4}D$$

if $|c_n|$ is greater than some constant A. For ψ_n to be a minimising sequence it is therefore necessary by (2.2) that $|c_n| \leqq A$ for all large enough n.

Theorem 2.2. *A stable ground state exists if*

$$\lim_{|x| \to \infty} V(x) = +\infty\,.$$

Proof. We assume that $V \geqq 0$, and copy the proof of the previous theorem until the last part. We deduce from (2.2) and (2.3) that

$$\min\{V(x-y-c_n) : x^2+y^2 \leqq B^2\} \leqq 2I_n \leqq 2(E+1)$$

which implies that the sequence c_n is bounded.

We next point out that stable ground states do not always exist. For any potential V which is strictly positive and vanishes at infinity it is clear that $c_n \to \infty$ for any minimising sequence ψ_n, so that there is no norm convergent subsequence. However, if the potential combines short range repulsion with long range attraction existence may be proved for large enough atomic masses. We conjecture that this restriction on the masses is also necessary.

Theorem 2.3. *Suppose that* $\lim_{|x| \to \infty} V(x) = 0$ *and that* $V(x) < 0$ *for some* $x \in \mathbb{R}^3$. *Then a stable ground state exists if* m_1 *and* m_2 *are large enough.*

Proof. Once again we modify only the last part of the proof of Theorem 2.1. If $c_n \to \infty$ then $I_n \to 0$ which implies that

$$\lim_{n \to \infty} \{\langle H\psi_n, \psi_n\rangle + \alpha W(\psi_n)\} = \lim_{n \to \infty} \left\langle \left(H_0 + \alpha \sum_{i=1}^{6} Q_i^2\right)\varphi_n, \varphi_n \right\rangle \geqq 0\,.$$

Thus the stable ground state exists if

$$\inf\{\langle H\psi,\psi\rangle+\alpha W(\psi):\|\psi\|=1\}<0.$$

But by taking ψ to be a C^∞ function with support in a small neighbourhood of the minimum of V we see that

$$\lim_{m_1,m_2\to\infty}\inf_{\|\psi\|=1}\{\langle H\psi,\psi\rangle+\alpha W(\psi)\}$$
$$=\min_{x\in\mathbb{R}^3}\{V(x)\}<0.$$

We mention, because of its possible computational value, that the above Theorems all have Hartree versions, where one minimises over wave functions $\psi=\psi_1\otimes\psi_2$ with $\psi_1,\psi_2\in L^2(\mathbb{R}^3)$.

Theorem 2.4. *If ψ minimises $\langle H\psi,\psi\rangle+\alpha W(\psi)$ subject to $\|\psi\|=1$ then*

$$H\psi+\alpha\sum_{i=1}^{6}\{Q_i^2\psi-2\langle Q_i\psi,\psi\rangle Q_i\psi\rangle=E\psi$$

for some real E, this equation being interpreted in the quadratic form sense on $Q(H)\cap\mathrm{Dom}\,W$.

Proof. If $\varphi\in Q(H)\cap\mathrm{Dom}(W)$ and $\langle\varphi,\psi\rangle=0$ and $\|\varphi\|=1$ then

$$\langle H(\psi\cos\theta+\varphi\sin\theta),\psi\cos\theta+\varphi\sin\theta\rangle+\alpha W(\psi\cos\theta+\varphi\sin\theta)$$
$$\geqq\langle H\psi,\psi\rangle+\alpha W(\psi)$$

for all real θ. Differentiating at $\theta=0$ we obtain

$$\langle H\psi,\varphi\rangle+\langle H\varphi,\psi\rangle+\alpha\sum_{i=1}^{6}\{\langle Q_i^2\psi,\varphi\rangle+\langle Q_i^2\varphi,\psi\rangle$$
$$-2\langle Q_i\psi,\psi\rangle\langle Q_i\psi,\varphi\rangle-2\langle Q_i\psi,\psi\rangle\langle Q_i\varphi,\psi\rangle\}=0.$$

Therefore if

$$\xi=H\psi+\alpha\sum_{i=1}^{6}\{Q_i^2\psi-2\langle Q_i\psi,\psi\rangle Q_i\psi\}$$

we see that

$$\langle\xi,\varphi\rangle+\langle\varphi,\xi\rangle=0$$

whenever $\langle\varphi,\psi\rangle=0$ and $\|\varphi\|=1$. This implies that $\xi=E\psi$ for some E.

We have now associated the functional

$$\langle H\psi,\psi\rangle+\alpha W(\psi)$$

with a non-linear Schrödinger equation (NLSE)

$$i\frac{\partial\psi}{\partial t}=H\psi+\alpha\sum_{i=1}^{6}\{Q_i^2\psi-2\langle Q_i\psi,\psi\rangle Q_i\psi\}. \tag{2.4}$$

It is easy to verify formally that any solution of this equation satisfies $\|\psi_t\| = 1$ for all t if it does so at $t=0$, and that

$$\langle H\psi_t, \psi_t\rangle + \alpha W(\psi_t)$$

is constant in time.

§ 3. Symmetry Breaking

Since both the Hamiltonian H and the weight W are invariant under the Euclidean group the uniqueness of the stable ground state of

$$\langle H\psi, \psi\rangle + \alpha W(\psi) \tag{3.1}$$

is intimately related to the question of symmetry breaking. Indeed even for the question of existence we had to break translational symmetry, since there are no translation invariant unit vectors in $\mathscr{H}$. For the rest of the section we assume that wave functions have centre of mass at the origin and consider only the problem of symmetry under the rotation group $SO(3)$.

It is clear that if the stable ground state ψ of (3.1) is unique then ψ is invariant under $SO(3)$. If $\alpha = 0$ the ground state (which is only square integrable after eliminating the centre of mass motion) is known to be non-degenerate for very general interactions between distinguishable atoms [11, p. 207]. On the other hand in quantum chemistry the molecular structure hypothesis allows one to talk about a molecule having a particular orientation with respect to the laboratory coordinates, and so suggests that the wave function of an unexcited molecule is not its quantum-mechanical ground state. Now it is to be expected that although the ground state is non-degenerate there are excited states whose energies differ from the ground state energy by an extremely small amount. It has been shown in [4, 5] for example that the difference between the first two energy levels of the anharmonic oscillator Hamiltonian

$$H = \frac{1}{2m} P^2 + \tfrac{1}{4}Q^4 - \tfrac{1}{2}Q^2$$

decreases very rapidly as $m \to \infty$, so that one has ground state degeneracy at $m = +\infty$. One therefore sees that superpositions of the lowest eigenstates of a molecular Hamiltonian may break rotational symmetry while being very nearly stationary in time.

The weakness of the above discussion is that no particular prescription is given for determining which superposition of the eigenstates is relevant for the problems of quantum chemistry. Our method resolves this difficulty at the cost of introducing a single undetermined parameter $\alpha > 0$.

We emphasise that unlike the ordinary anharmonic oscillator [1, 4, 5] the ground state degeneracy of the following theorem occurs for finite values of the atomic masses.

Theorem 3.1. *Suppose that the potential V takes its minimum value A only when $|x| = r_0 > 0$. Then the stable ground state of H with centre of mass at the origin is not unique and breaks rotational symmetry provided the atomic masses are large enough.*

Proof. If ψ has centre of mass at the origin and is spherically symmetric then $\langle Q_i\psi, \psi\rangle = 0$ for all i. Hence

$$\langle H\psi, \psi\rangle + \alpha W(\psi) = \left\langle \left(H + \alpha \sum_{i=1}^{6} Q_i^2\right)\psi, \psi \right\rangle$$
$$\geqq \min\{V(x-y) + \alpha x^2 + \alpha y^2 : x, y \in \mathbb{R}^3\} \equiv A'.$$

However as we have already shown

$$\lim_{m_1, m_2 \to \infty} [\min\{\langle H\psi, \psi\rangle + \alpha W(\psi) : \|\psi\| = 1\} = A$$

and the hypothesis on V implies that $A < A'$.

The symmetry breaking above is associated with a phase transition. Namely the parameter space

$$\{m_1, m_2, \alpha) : m_1 > 0, m_2 > 0, \alpha > 0\}$$

may be divided into two regions depending on whether the ground state is unique or not. For any $\alpha > 0$ it is not unique for sufficiently large m_1 and m_2. It seems likely that for any $\alpha > 0$ the ground state is unique for small enough m_1 and m_2, but we do not have a general proof.

To clarify the position we analyse in some detail a simple example, which is probably fairly typical. We consider two atoms of equal mass interacting anharmonically in one dimension with Hamiltonian

$$H = \frac{1}{2m} P_1^2 + \frac{1}{2m} P_2^2 + \tfrac{1}{4}(Q_1 - Q_2)^4 - \tfrac{1}{2}(Q_1 - Q_2)^2.$$

The explicit expression for W is

$$W(\psi) = \langle Q_1^2\psi, \psi\rangle + \langle Q_2^2\psi, \psi\rangle - \langle Q_1\psi, \psi\rangle^2 - \langle Q_2\psi, \psi\rangle^2.$$

We consider the breaking of reflection symmetry, where

$$(R\psi)(x) = \psi(-x)$$

in the case $\alpha = 1$. It is useful to define $K = \frac{1}{2}P^2 + Q^4$ and to denote its eigenvalues in increasing order by $E_0, E_1, \ldots$ and the corresponding normalised eigenvectors by $\psi_0, \psi_1, \ldots$.

Theorem 3.2. *The functional $\langle H\psi, \psi\rangle + W(\psi)$ has a unique minimum subject to $\|\psi\| = 1$ and*

$$\langle Q_1\psi, \psi\rangle + \langle Q_2\psi, \psi\rangle = 0 \tag{3.2}$$

if and only if

$$\langle K\psi, \psi\rangle - m^{1/3}\langle Q\psi, \psi\rangle^2 > E_0 \tag{3.3}$$

for all unit vectors $\psi \in L^2(\mathbb{R})$ such that $\psi \neq \psi_0$.

Proof. Because the centre of mass is at the origin

$$\langle H\psi, \psi\rangle + W(\psi)$$
$$= \langle (H + Q_1^2 + Q_2^2)\psi, \psi\rangle - \tfrac{1}{2}\langle (Q_1 - Q_2)\psi, \psi\rangle^2$$

which on rotating coordinates may be written as

$$\left\langle \left(\frac{1}{2m} P_1^2 + \frac{1}{2m} P_2^2 + Q_1^4 + Q_2^2 \right) \psi, \psi \right\rangle - \langle Q_1 \psi, \psi \rangle^2$$

and then by a scale transformation as

$$m^{-2/3} \langle K_1 \psi, \psi \rangle + m^{-1/2} \langle (\tfrac{1}{2} P_2^2 + Q_2^2) \psi, \psi \rangle - m^{-1/3} \langle Q_1 \psi, \psi \rangle^2 . \tag{3.4}$$

Let F_n denote the eigenvalues of $(\frac{1}{2} P^2 + Q^2)$ in increasing order and φ_n the corresponding normalised eigenvectors. If (3.4) has a unique minimum subject to the condition $\langle Q_2 \psi, \psi \rangle = 0$, which corresponds to (3.2), then by reflection symmetry the minimum satisfies $\langle Q_1 \psi, \psi \rangle = 0$ which implies that $\psi = \psi_0 \otimes \varphi_0$. We therefore have to determine whether

$$\langle K_1 \psi, \psi \rangle + m^{1/6} \langle (\tfrac{1}{2} P_2^2 + Q_2^2) \psi, \psi \rangle - m^{1/3} \langle Q_1 \psi, \psi \rangle^2 > E_0 + m^{1/6} F_0 \tag{3.5}$$

for all unit vectors $\psi \neq \psi_0 \otimes \varphi_0$ with $\langle Q_2 \psi, \psi \rangle = 0$.

Now $\psi = \sum \alpha_n \xi_n \otimes \varphi_n$ where $\|\xi_n\| = 1$ and $\sum |\alpha_n|^2 = 1$, so

$$\begin{aligned}
&\langle K_1 \psi, \psi \rangle + m^{1/6} \langle (\tfrac{1}{2} P_2^2 + Q_2^2) \psi, \psi \rangle - m^{1/3} \langle Q_1 \psi, \psi \rangle^2 \\
&\quad = \sum |\alpha_n|^2 \langle K \xi_n, \xi_n \rangle + m^{1/6} \sum F_n |\alpha_n|^2 - m^{1/3} \{ \sum |\alpha_n|^2 \langle Q \xi_n, \xi_n \rangle \}^2 \\
&\quad \geqq \sum |\alpha_n|^2 \langle K \xi_n, \xi_n \rangle + m^{1/6} \sum F_n |\alpha_n|^2 - m^{1/3} \sum |\alpha_n|^2 \langle Q \xi_n, \xi_n \rangle^2 \\
&\quad \geqq \sum |\alpha_n|^2 \{ \langle K \xi_n, \xi_n \rangle + m^{1/6} F_0 - m^{1/3} \langle Q \xi_n, \xi_n \rangle^2 \}
\end{aligned}$$

with strict inequality unless $\alpha_0 = 1$ and $\alpha_n = 0$ for all $n \geqq 1$.

Therefore (3.3) implies (3.5) unless $\alpha_0 = 1$, $\alpha_n = 0$ for all $n \geqq 1$ and $\xi_0 = \psi_0$, that is unless $\psi = \psi_0 \otimes \varphi_0$. The converse is similar.

We have already shown that reflection symmetry is broken for large enough m. It is easy to use Theorem 3.2 to obtain upper bounds on the critical mass. For example if ψ_a denotes the translate of ψ_0 by a distance a then

$$\begin{aligned}
&\langle K \psi_a, \psi_a \rangle - m^{1/3} \langle Q \psi_a, \psi_a \rangle^2 \\
&\quad = \langle \{ \tfrac{1}{2} P^2 + (Q + a)^4 \} \psi_0, \psi_0 \rangle - m^{1/3} \langle (Q + a) \psi_0, \psi_0 \rangle^2 \\
&\quad = E_0 + 6a^2 \langle Q^2 \psi_0, \psi_0 \rangle + a^4 - m^{1/3} a^2
\end{aligned}$$

which is less than E_0 for small a if

$$m^{1/3} > 6 \langle Q^2 \psi_0, \psi_0 \rangle .$$

We next prove that reflection symmetry is not broken for small masses.

Theorem 3.3. *If*

$$m^{1/3} < (E_1 - E_0)/2(1 + E_1)$$

then the stable ground state is unique subject to having its centre of mass at the origin.

Proof. Write $\psi = u \psi_0 + v \varphi$ where $\|\varphi\| = 1$, $\langle \varphi, \psi_0 \rangle = 0$ and $|u|^2 + |v|^2 = 1$.

Since $\langle Q \psi_0, \psi_0 \rangle = 0$

$$\begin{aligned}
|\langle Q \psi, \psi \rangle| &= |uv \langle Q \psi_0, \varphi \rangle + v \langle Q \varphi, \psi \rangle| \\
&\leqq 2|v| \, \|Q \varphi\|
\end{aligned}$$

so

$$\begin{aligned}\langle Q\psi,\psi\rangle^2 &\leqq 4|v|^2\langle Q^2\varphi,\varphi\rangle\\ &\leqq 2|v|^2\{\langle Q^4\varphi,\varphi\rangle+1\}\\ &\leqq 2|v|^2\{\langle K\varphi,\varphi\rangle+1\}.\end{aligned}$$

Therefore

$$\begin{aligned}&\langle K\psi,\psi\rangle-m^{1/3}\langle Q\psi,\psi\rangle^2\\ &\quad\geqq |u|^2E_0+|v|^2\langle K\varphi,\varphi\rangle-2m^{1/3}|v|^2\{\langle K\varphi,\varphi\rangle+1\}\\ &\quad\geqq |u|^2E_0+|v|^2[(1-2m^{1/3})E_1-m^{1/3}2]\end{aligned}$$

which is greater than E_0 if $v\neq 0$ and

$$(1-2m^{1/3})E_1-2m^{1/3}>E_0\,.$$

While quantitatively poor, the above theorems establish that there is a critical mass $0<\bar{m}<\infty$ such that if $m>\bar{m}$ the minimum is not unique and breaks reflection symmetry, while if $m<\bar{m}$ the unique minimum is equal to ψ_0.

We now describe a technique which enables one to determine $\bar{m}$ to any degree of accuracy. Let L_n be the linear span of $\psi_0,\ldots,\psi_{n-1}$ and let $\bar{m}_n$ be the largest mass for which

$$\langle K\psi,\psi\rangle-m^{1/3}\langle Q\psi,\psi\rangle^2$$

has a unique minimum, necessarily at ψ_0, in the subspace L_n. We consider the constants $\bar{m}_n$ to be computable since they depend on finding the minimum of a continuous function on the unit ball of $\mathbb{C}^n$. For example

$$\bar{m}_2=4^{-3}(E_1-E_0)^3\langle Q\psi_0,\psi_1\rangle^{-6}.$$

It is clear from their definition that $\bar{m}_n$ decrease monotonically as $n\to\infty$. Moreover since $\mathrm{lin}\{\psi_n\}$ is a quadratic form core for K, it is easy to verify that

$$\lim_{n\to\infty}\bar{m}_n=\bar{m}\,. \tag{3.6}$$

The point of the following theorem is that it controls the rate of convergence in (3.6).

Theorem 3.4. *If ε_n is defined by*

$$8(\bar{m}_2)^{2/3}(1+\varepsilon_n^{-1})^2=\tfrac{1}{2}E_n-E_0$$

then

$$\bar{m}_n\geqq\bar{m}\geqq(1+\varepsilon_n)^{-3}\bar{m}_n\,.$$

Proof. If $\|\psi\|=1$ we may write $\psi=u\xi+v\eta$ where $\|\xi\|=1$, $\|\eta\|=1$, $\xi\in L_n$, $\eta\in L_n^{\perp}$ and $|u|^2+|v|^2=1$. Then

$$\begin{aligned}|\langle Q\psi,\psi\rangle| &= |\,|u|^2\langle Q\xi,\xi\rangle+u\bar{v}\langle Q\xi,\eta\rangle+v\langle Q\eta,\psi\rangle|\\ &\leqq |u\langle Q\xi,\xi\rangle|+2|v|\,\|Q\eta\|\,.\end{aligned}$$

Therefore

$$\langle Q\psi,\psi\rangle^2 \leqq (1+\varepsilon)|u|^2\langle Q\xi,\xi\rangle^2+(1+\varepsilon^{-1})4|v|^2\langle Q^2\eta,\eta\rangle$$
$$\leqq (1+\varepsilon)|u|^2\langle Q\xi,\xi\rangle^2+(1+\varepsilon^{-1})|v|^2\{\lambda\langle K\eta,\eta\rangle+4\lambda^{-1}\}$$

for any $\varepsilon,\lambda>0$. It follows that

$$\langle K\psi,\psi\rangle - m^{1/3}\langle Q\psi,\psi\rangle^2$$
$$\geqq |u|^2\{\langle K\xi,\xi\rangle-(1+\varepsilon)m^{1/3}\langle Q\xi,\xi\rangle^2\}$$
$$+|v|^2\{\langle K\eta,\eta\rangle-(1+\varepsilon^{-1})m^{1/3}\{\lambda\langle K\eta,\eta\rangle+4\lambda^{-1}\}\}.$$

Putting

$$\lambda=\tfrac{1}{2}m^{-1/3}(1+\varepsilon^{-1})^{-1}$$

and noting that $\langle K\eta,\eta\rangle\geqq E_n$, we see that the minimum is unique provided

$$(1+\varepsilon)^3 m<\bar{m}_n$$

and

$$\tfrac{1}{2}E_n-8m^{2/3}(1+\varepsilon^{-1})^2>E_0.$$

These estimates are implied by the pair

$$(1+\varepsilon)^3 m<\bar{m}_n$$

and

$$\tfrac{1}{2}E_n-8(\bar{m}_2)^{2/3}(1+\varepsilon^{-1})^2=E_0.$$

This yields the stated lower bound on $\bar{m}$, the upper bound being trivial.

§ 4. An Exactly Soluble Non-linear Schrödinger Equation

Our discussion in Sect. 2 led us to the NLSE (2.4), which is of some interest in its own right. Such equations raise many interesting problems at the foundations of quantum mechanics. For example one has to reconsider ab initio the definition of mixed states [10], macroscopic causality [3] and the measurement problem [6]. One of the main difficulties concerns scale invariance, that is whether $H(\lambda\psi)=\lambda H(\psi)$ for all $\lambda\in\mathbb{C}$. This can be achieved for our problem by redefining

$$W(\psi)=\sum_{i=1}^{6}\{\langle Q_i^2\psi,\psi\rangle-\langle Q_i\psi,\psi\rangle^2/\|\psi\|^2\}$$

which necessitates no changes in our above results because we always assumed that $\|\psi\|=1$.

In this section we study the "free" one-particle NLSE on $L^2(\mathbb{R}^3)$ which, after normalisation, may be written as

$$i\frac{\partial\psi}{\partial t}=-\tfrac{1}{2}\Delta\psi+\tfrac{1}{2}x^2\psi-\sum_{i=1}^{3}\frac{\langle Q_i\psi,\psi\rangle}{\langle\psi,\psi\rangle}x_i\psi. \tag{4.1}$$

We let $\mathscr{L}$ denote the quadratic form domain of the harmonic oscillator

$$\mathscr{L} = \{\psi : \langle -\tfrac{1}{2}\Delta\psi + \tfrac{1}{2}x^2\psi, \psi\rangle < \infty\}$$

and for $p, q \in \mathbb{R}^3$ define

$$\mathscr{L}_{pq} = \{\psi \in \mathscr{L} : \langle Q\psi, \psi\rangle = q \text{ and } \langle P\psi, \psi\rangle = p\}.$$

Note that $\mathscr{L}_{pq}$ is a subset of $\mathscr{L}$ but not a linear subspace.

Theorem 4.1. *For all $\varphi \in \mathscr{L}$ there is a unique solution $\varphi_t = U_t\varphi$ of the* NLSE (4.1) *such that $\varphi_t \in \mathscr{L}$ for all t. Moreover U_t maps $\mathscr{L}_{pq}$ onto $\mathscr{L}_{p,q+pt}$ and coincides on $\mathscr{L}_{pq}$ with a linear unitary operator.*

Proof. Given any solution one verifies that

$$\langle P\psi_t, \psi_t\rangle = \langle P\psi_0, \psi_0\rangle$$
$$\langle Q\psi_t, \psi_t\rangle = \langle Q\psi_0, \psi_0\rangle + t\langle P\psi_0, \psi_0\rangle$$

so that one can rewrite the NLSE as

$$i\frac{\partial\psi}{\partial t} = -\tfrac{1}{2}\Delta\psi + \tfrac{1}{2}x^2\psi - \sum_{i=1}^{3}(q_i + p_i t)x_i\psi.$$

But this is a linear Schrödinger equation which is exactly soluble for $\psi \in \mathscr{L}_{pq}$. For notational simplicity we write down the solution only in one space dimension.

If

$$i\frac{\partial\psi}{\partial t} = -\tfrac{1}{2}\frac{\partial^2\psi}{\partial x^2} + \tfrac{1}{2}x^2\psi - (q + pt)x\psi \tag{4.2}$$

and we define

$$\varphi(x) = (U_{pqt}\psi)(x) \equiv e^{-ipx - i\theta(p,q,t)}\psi(x + q + pt)$$

then a straightforward computation shows that

$$i\frac{\partial\varphi}{\partial t} = -\tfrac{1}{2}\frac{\partial^2\varphi}{\partial x^2} + \tfrac{1}{2}x^2\varphi$$

for a suitable choice of the phase function $\theta(p, q, t)$. Putting $H = \frac{1}{2}(P^2 + Q^2)$ we see that the solution of (4.2) is

$$\psi_t = U^*_{p,q,t}e^{-tH}U_{p,q,0}\psi_0.$$

The fact that the evolution operator $U_t : \mathscr{L}_{pq} \to \mathscr{L}_{p,q+pt}$ is essentially linear, together with the observation that each $\mathscr{L}_{pq}$ is a dense subset of $\mathscr{H}$, allows one to extend U_t from $\mathscr{L}_{pq}$ to a unitary operator on $\mathscr{H}$. This is not a good idea however, since one gets a different extension for each choice of p, q, as indeed one must because of the nonlinearity of the original Schrödinger equation. The point is that although the solutions of the NLSE satisfy $\|U_t\psi\| = \|\psi\|$ for all $\psi \in \mathscr{L}$ and $t \in \mathbb{R}$, there is no way of extending U_t to a continuous map on the whole of $\mathscr{H}$. Apart from a special class of states discussed below, it seems that the NLSE makes sense only for $\psi \in \mathscr{L}$. One may summarise the nature of the NLSE by describing

$\mathscr{L} = \bigcup_{pq} \mathscr{L}_{pq}$ as a fibre bundle with fibres $\mathscr{L}_{pq}$ and base space $\mathbb{R}^6$, and U_t as a one-parameter group of fibre bundle automorphisms of $\mathscr{L}$.

Theorem 4.2. *For each $p, q \in \mathbb{R}^3$ and $n \in \mathbb{Z}_3^+$ there exist solitary wave solutions of the* NLSE *with position q at time zero, momentum p and excitation number n.*

Proof. If φ_n is the nth excited state of the harmonic oscillator then

$$\langle P\varphi_n, \varphi_n \rangle = \langle Q\varphi_n, \varphi_n \rangle = 0 .$$

Therefore

$$\psi_t = U_{pqt}^* e^{-iHt} \varphi_n$$

is a solution of the NLSE. But since φ_n is an eigenvector of H

$$\psi_t(x) = e^{-i(|n|+3/2)t} \{U_{pqt}^* \varphi_n\}(x)$$

so

$$|\psi_t(x)|^2 = |\varphi_n(x-q-pt)|^2$$

as required for a solitary wave.

The space reflection $(R\psi)(x) = \psi(-x)$ may be used to produce another simple class of solutions of the NLSE. If $\psi \in \mathscr{H}$ then there is at most one pair (p, q) such that

$$RU_{pq0}\psi = \pm U_{pq0}\psi . \tag{4.3}$$

If $\psi \in \mathscr{L}$ and if (4.3) holds then

$$p = \langle P\psi, \psi \rangle ; \quad q = \langle Q\psi, \psi \rangle$$

but (4.3) can serve to define the position and momentum of certain states which do not lie in $\mathscr{L}$. For such ψ one may define

$$\psi_t = U_{pqt}^* e^{-iHt} U_{pq0}\psi$$

as generalised solutions of the NLSE.

§ 5. Generalisations of the NLSE

The non-linear Schrödinger equation of Sect. 4 possesses solitary waves which move classically with momentum p and position $(q+pt)$. These waves also possess internal excitations which evolve as for the harmonic oscillator. One may interpret these excitations as internal structure of the particle induced by the non-linearity, or, more plausibly, as oscillations due to the medium in which the particle is travelling.

It is natural to ask to what extent these results depend upon the precise form (4.1) of the NLSE. In this section we investigate this problem for a NLSE in one dimension, of the general form

$$i\frac{\partial \psi}{\partial t} = \frac{1}{2m} P^2 \psi + V(\psi) \tag{5.1}$$

where

$$V(\psi)=\sum_{r=0}^{n}\alpha_r(\psi)Q^r\psi$$

and $\psi\in L^2(\mathbb{R})$, $\alpha_r: L^2(\mathbb{R})\to\mathbb{R}$ being homogeneous of degree zero to ensure scale invariance of the NLSE.

We let U_a be the space translation

$$(U_a\psi)(x)=\psi(x-a)$$

and for the sake of precision assume that there is a dense linear subspace $\mathscr{L}$ in $L^2(\mathbb{R})$ which contains C_c^∞, is invariant under all U_a and has the further property that for all $\psi\in\mathscr{L}$, (5.1) has a unique solution within $\mathscr{L}$ for all $t\in\mathbb{R}$.

Lemma 5.1. *If ψ_t is a solution of* (5.1) *in $\mathscr{L}$ then*

$$\frac{\partial}{\partial t}\langle Q\psi_t,\psi_t\rangle=\frac{1}{m}\langle P\psi_t,\psi_t\rangle$$

$$\frac{\partial}{\partial t}\langle P\psi_t,\psi_t\rangle=-\sum_{r=0}^{n}r\alpha_r(\psi_t)\langle Q^{r-1}\psi_t,\psi_t\rangle.$$

The NLSE *is invariant under space translations if and only if*

$$\alpha_s(\psi)=\sum_{r=s}^{n}\binom{r}{s}a^{r-s}\alpha_r(U_a\psi) \tag{5.2}$$

for all $a\in\mathbb{R}$, $\psi\in\mathscr{L}$ and $s=0,\ldots,n$.

Proof. The first two results are straightforward computations. For the third we note that space translation invariance is dependent upon

$$U_a\left(\frac{1}{2m}P^2\psi+\sum_{r=0}^{n}\alpha_r(\psi)Q^r\psi\right)=\frac{1}{2m}P^2U_a\psi+\sum_{r=0}^{n}\alpha_r(U_a\psi)Q^rU_a\psi$$

or equivalently

$$\sum_{s=0}^{n}\alpha_s(\psi)Q^s\psi=\sum_{r=0}^{n}\alpha_r(U_a\psi)U_{-a}Q^rU_a\psi=\sum_{r=0}^{n}\alpha_r(U_a\psi)(Q+a)^r\psi$$

which may be rewritten as

$$\sum_{s=0}^{n}\alpha_s(\psi)Q^s\psi=\sum_{s=0}^{n}\sum_{r=s}^{n}\alpha_r(U_a\psi)\binom{r}{s}a^{r-s}Q^s\psi.$$

Equation (5.2) then results from the fact that $\psi, Q\psi,\ldots,Q^n\psi$ are linearly independent in $L^2(\mathbb{R})$ if $\psi\neq 0$.

It is important to realise that space translation invariance does not imply the conservation of momentum

$$\frac{\partial}{\partial t}\langle P\psi_t,\psi_t\rangle=0$$

in the non-linear case. As a simple example consider

$$i\frac{\partial\psi}{\partial t}=\frac{1}{2m}P^2\psi+Q\psi-\frac{\langle Q\psi,\psi\rangle}{\langle\psi,\psi\rangle}\psi$$

which describes a particle moving with constant acceleration.

Theorem 5.2. *Suppose that the* NLSE (5.1) *is translationally invariant. If* $\frac{\partial\psi}{\partial t}$ *is a linear function of* ψ *on the (nonlinear) subset*

$$\mathscr{L}_0=\{\psi\in\mathscr{L}:\langle Q\psi,\psi\rangle=0\}$$

of $\mathscr{L}$, *in the sense that* $\alpha_r(\psi)$ *are constant on* $\mathscr{L}_0$, *then*

$$V(\psi)=\sum_{r=0}^{n}c_r\left\{Q-\frac{\langle Q\psi,\psi\rangle}{\langle\psi,\psi\rangle}\right\}^r\psi \tag{5.3}$$

for all $\psi\in\mathscr{L}$ *and some* $c_0,\ldots,c_n\in\mathbb{R}$.

Proof. We put $\varphi=U_a\psi$ where $a=-\langle Q\psi,\psi\rangle/\langle\psi,\psi\rangle$. Then $\langle Q\varphi,\varphi\rangle=0$ so $\varphi\in\mathscr{L}_0$ and the linearity assumption implies that

$$\alpha_r(\varphi)=c_r \tag{5.4}$$

for some constants $c_0,\ldots,c_n$ independent of φ. Now Eq. (5.2) leads to the formula

$$\alpha_s(\psi)=\sum_{r=s}^{n}\binom{r}{s}a^{r-s}c_r$$

and hence to

$$\begin{aligned}V(\psi)&=\sum_{s=0}^{n}\sum_{r=s}^{n}\binom{r}{s}a^{r-s}c_rQ^s\psi\\&=\sum_{r=0}^{n}c_r(Q+a)^r\psi\\&=\sum_{r=0}^{n}c_r\left\{Q-\frac{\langle Q\psi,\psi\rangle}{\langle\psi,\psi\rangle}\right\}^r\psi.\end{aligned}$$

Theorem 5.3. *If in addition to the above conditions, the subset*

$$\mathscr{L}_{00}=\{\psi\in\mathscr{L}:\langle Q\psi,\psi\rangle=\langle P\psi,\psi\rangle=0\}$$

is invariant under the time evolution then

$$V(\psi)=c_2\left\{Q-\frac{\langle Q\psi,\psi\rangle}{\langle\psi,\psi\rangle}\right\}^2\psi+c_0\psi$$

for some $c_0,\ c_2\in\mathbb{R}$.

Proof. By Lemma 5.1 the subset $\mathscr{L}_{00}$ is invariant if and only if

$$\sum_{r=0}^{n}r\alpha_r(\psi)\langle Q^{r-1}\psi,\psi\rangle=0$$

for all $\psi\in\mathscr{L}_{00}$, which necessitates $c_r=0$ unless $r=0$ or $r=2$.

This last theorem provides a degree of post hoc justification for our original choice of W. While much of Sects. 2 and 3 can be reproduced for other similar choices of W, it seems likely that further developments, for example of scattering theory, will depend upon the explicit solubility of the single particle problem. The theorem states that the W chosen in Sect. 1 is the only one of polynomial type for which the NLSE has space translation invariance, conservation of momentum and exact solubility in the sense of linearity of the Hamiltonian on $\mathscr{L}_0$ (as defined in Theorem 5.2).

§ 6. Quantisation of the Medium

Since the non-linearity of our Schrödinger equation was motivated by reference to the polarisation of a medium in which the atom is travelling, one might hope that by explicitly introducing that medium in second quantised form one could recover the NLSE.

Noting the analogy between Choquard's functional

$$\mathscr{E}_0(\varphi)=\frac{1}{2m}\int|\nabla\varphi|^2dx-\alpha\iint|\varphi(x)|^2|x-y|^{-1}|\varphi(y)|^2dxdy$$

and ours, written in the form

$$\mathscr{E}(\varphi)=\frac{1}{2m}\int|\nabla\varphi|^2dx+\frac{\alpha}{2}\iint|\varphi(x)|^2(x-y)^2|\varphi(y)|^2dxdy$$

one can write down an appropriate second quantised linear Hamiltonian, which is a modification of that describing the polaron (see [9] and references cited there).

We define

$$H=H_a+H_b+H_I$$

where

$$H_a=-\frac{1}{2m}\Delta$$

and

$$H_b=\omega\int a(k)^*a(k)dk$$

$a^{\#}(k)$ being the creation-annihilation operators of a phonon field at the point k of momentum space. We define

$$H_I=\int f(k)\{a(k)^*e^{-ik.x}+a(k)e^{ik.x}\}dk$$

where we assume that f is spherically symmetric and

$$\int|f(k)|^2(1+k^2)dk<\infty\,. \tag{6.1}$$

An upper bound to the ground state energy of H may be obtained by using states of the Hartree type, namely $\psi=\psi_a\otimes\psi_b$ where ψ_a is an atomic state and ψ_b a state of the phonon field, both being of unit norm.

Theorem 6.1. *The quantity*

$$\langle H\psi_a \otimes \psi_b, \psi_a \otimes \psi_b \rangle \tag{6.2}$$

is minimised by taking ψ_b to be a coherent phonon state and ψ_n an atomic state which minimises

$$\mathscr{E}_1(\psi) = \frac{1}{2m}\int |\nabla\psi|^2 dx - \omega^{-1}\iint \sigma(x-y)|\psi(x)|^2|\psi(y)|^2 dxdy$$

where

$$\sigma(x) = \int |f(k)|^2 e^{ix.k} dk\,. \tag{6.3}$$

Proof. If we define $\hat{\varrho}(k)$ to be the Fourier transform of

$$\varrho(x) = |\psi_a(x)|^2$$

then a direct computation shows that

$$\langle H\psi_a \otimes \psi_b, \psi_a \otimes \psi_b \rangle = -\frac{1}{2m}\langle \Delta\psi_a, \psi_a \rangle$$
$$+ \langle \int \{\omega a(k)^* a(k) + g(k)a(k)^* + g(\bar{k})a(k)\} dk\psi_b, \psi_b \rangle$$

where

$$g(k) = f(k)\hat{\varrho}(k)$$

lies in $L^2(\mathbb{R}^3)$. For fixed ψ_a the ground state of the phonon term is a coherent state with energy

$$E = -\omega^{-1}\int |g(k)|^2 dk$$
$$= -\omega^{-1}\int |f(k)|^2 |\hat{\varrho}(k)|^2 dk$$
$$= -\omega^{-1}\iint \sigma(x-y)\varrho(x)\varrho(y) dxdy\,.$$

So if we minimise (6.2) first with respect to ψ_b and then with respect to ψ_a we obtain the stated result.

It is formally clear that for large atomic mass m, $\mathscr{E}_1(\psi)$ should be minimised for a state which is concentrated in a very small region in space. But if $(x-y)$ is very small

$$\sigma(x-y) \doteqdot \beta - \frac{\alpha}{2}(x-y)^2$$

by (6.1) and (6.3), with $\alpha, \beta \geqq 0$. Therefore for large atomic masses $\mathscr{E}_1(\psi)$ is approximately equal to

$$\mathscr{E}_2(\psi) = \frac{1}{2m}\int |\nabla\psi|^2 dx - \omega^{-1}\iint \left\{\beta - \frac{\alpha}{2}(x-y)^2\right\} |\psi(x)|^2 |\psi(y)|^2 dxdy$$
$$= \frac{1}{2m}\int |\nabla\psi|^2 dx + \alpha\omega^{-1} W(\psi) - \beta\omega^{-1}\|\psi\|^2$$

which is the expression we started with, up to a self-energy renormalisation $\beta\omega^{-1}$.

The above discussion produces a relationship between the Hamiltonian H and the weight W, but little more. It is unclear why one should minimise $\langle H\psi, \psi\rangle$ only for states ψ of Hartree type, and whether this gives the ground state energy (or more precisely the bottom of the spectrum of H, which possesses no bound states) exactly in the asymptotic limit $m\to\infty$. It also remains to be seen whether there is a similar relationship between the dynamics for H and for the NLSE.

The following discussion shows that such a dynamic relationship must necessarily be asymptotic not exact. We define solitary waves with respect to a Schrödinger equation

$$i\frac{\partial\psi}{\partial t} = H(\psi) \tag{6.4}$$

on a Hilbert space $\mathscr{H}$ to be a family of unit vectors $\psi_{pq}\in\mathscr{H}$ with the following properties

(i) The solution of (6.4) at time t with initial state ψ_{pq} is of the form

$$e^{i\theta(p,q,t)}\psi_{p,q+pt}.$$

(ii) ψ_{pq} and $\psi_{p'q'}$ are linearly independent unless $p=p'$ and $q=q'$.

(iii) ψ_{pq} depends norm continuously on p, q.

Theorem 6.2. *No linear Schrödinger equation possesses solitary waves.*

Proof. Given $q\neq 0$ let

$$a=\min_{\theta\in\mathbb{R}}\|\psi_{00}-e^{i\theta}\psi_{0q}\|>0.$$

Using (iii) let $|p|<\delta$ imply

$$\|\psi_{00}-\psi_{p0}\|<\frac{a}{2};\quad \|\psi_{0q}-\psi_{pq}\|<\frac{a}{2}.$$

Now choose p and $t>0$ so that $q=pt$ and $|p|<\delta$. Then by (i) if H is linear

$$\psi_{pq}=e^{-i\theta}e^{-iHt}\psi_{p0}$$

and

$$\psi_{00}=e^{-i\varphi}e^{-iHt}\psi_{00}$$

so

$$\begin{aligned}\|\psi_{0q}-e^{i(\varphi-\theta)}\psi_{00}\| &= \|(\psi_{0q}-\psi_{pq})+e^{-i\theta}e^{-iHt}(\psi_{p0}-\psi_{00})\|\\ &\leqq \|\psi_{0q}-\psi_{pq}\|+\|\psi_{p0}-\psi_{00}\|<a\end{aligned}$$

contrary to the definition of a.

We finally mention a conjecture about how solitary waves may occur for the second quantised Schrödinger equation in spite of the above theorem. First recall that since the medium has an infinite number of degrees of freedom, no single Hilbert space representation is adequate to describe all its excitations. It is possible that the polarisation of the medium due to the atom is so substantial that each solitary wave of the NLSE is associated with an inequivalent representation of the

CCR algebra for the medium. In this case Theorem 6.2 would not be applicable since the states ψ_{pq} would all lie in orthogonal Hilbert spaces and condition (iii) would not hold.

§ 7. A Simplified Nuclear Shell Model

In this section we give another "derivation" of the NLSE for a model Hamiltonian of a type which is popular in the analysis of nuclear structure. For simplicity we assume that we have n nucleons of mass m and spin zero moving in one space dimension. If the nucleons have wave functions $\varphi_r \in L^2(\mathbb{R})$ and are attracted harmonically to their collective centre of mass then their equations of motion are defined in the model as

$$i\frac{\partial \varphi_r}{\partial t} = \frac{1}{2m} P_r^2 \varphi_r + \frac{\omega^2}{2} \{Q_r - q(t)\}^2 \varphi_r \tag{7.1}$$

where

$$q(t) = \frac{1}{n} \sum_{r=1}^{n} \langle Q_r \varphi_r, \varphi_r \rangle . \tag{7.2}$$

Theorem 7.1. *If* $\psi = \bigotimes_{r=1}^{n} \varphi_r$ *then the dynamical Eqs.* (7.1) *and* (7.2) *are equivalent to*

$$i\frac{\partial \psi}{\partial t} = \frac{1}{2m} \sum_{r=1}^{n} P_r^2 \psi + \frac{\omega^2}{4n} \sum_{r,s} (Q_r - Q_s)^2 \psi + \frac{n\omega^2}{2} \{\bar{Q} - \langle \bar{Q}\psi, \psi \rangle\}^2 \psi \tag{7.3}$$

where

$$\bar{Q} = \frac{1}{n} \sum_{r=1}^{n} Q_r .$$

Proof. This is a consequence of the well-known identity

$$\sum_{r=1}^{n} \{Q_r - q(t)\}^2 = \frac{1}{2n} \sum_{r,s} (Q_r - Q_s)^2 + n\{\bar{Q} - q(t)\}^2$$

and together with

$$q(t) = \langle \bar{Q}\psi, \psi \rangle .$$

While mathematically trivial, the theorem is interesting in that Eq. (7.3) can be interpreted as arising from a harmonic potential between all pairs of nucleons together with a nonlinear term of the usual type acting on the centre of mass. If the internal degrees of freedom are separated in the usual manner then the centre of mass evolves according to our NLSE.

Since (7.1) is a *linear* time-dependent Schrödinger equation. $\varphi_1, \ldots, \varphi_n$ are orthogonal for all times if they are so at time zero. Thus there is no problem in accommodating Fermion statistics.

We see as in the previous section that the NLSE seems to be theoretically related to the Hartree condition. It would be valuable to find a deeper explanation of this phenomenon.

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