Nonlinear interference in a mean-field quantum model

Gilbert Reinisch\textsuperscript{1} and Vidar Gudmundsson\textsuperscript{2}
\textsuperscript{1}Université de Nice - Sophia Antipolis, CNRS, Observatoire de la Côte d’Azur, BP 4229, 06304 - Nice Cédex 4, France
\textsuperscript{2}Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland

Using similar nonlinear stationary mean-field models for Bose-Einstein Condensation of cold atoms and interacting electrons in a Quantum Dot, we propose to describe the original many-particle ground state as a one-particle statistical mixed state of the nonlinear eigenstates whose weights are provided by the eigenstate non-orthogonality. We search for physical grounds in the interpretation of our two main results, namely, quantum-classical nonlinear transition and interference between nonlinear eigenstates.

PACS numbers: 73.21.La 71.10.Li 71.90+q

I. INTRODUCTION

Commonly, quantum mechanical models of many interacting particles – linear models – are made computationally tractable by transforming them into a mean-field single-particle models, at the cost of making the model nonlinear, but solvable \cite{1}. Yet, solvable has a different meaning within two fields of condensed matter physics, the field of cold atoms in an external trap, and the field of electrons in a quantum dot. In the former field, the ensuing equation for the Bose-Einstein condensate (BEC), namely, the Gross-Pitaevskii equation (GPE), is often solved directly as a nonlinear differential equation \cite{2} \cite{3}. In the latter case, for electrons confined in a quantum dot, the approximation applied for the Coulomb interaction between the electrons leads to the Hartree, the Hartree-Fock, or Kohn-Sham type of an equation. All these are nonlinear equations that are conventionally solved by an iteration scheme. These equations for the electrons have a similar nonlinear term as for the GPE, but the long range nature of the Coulomb interaction makes them more complex. Within each iteration, the mean-field potential is constructed with information about the charge distribution and/or the wave functions from former iterations. The nonlinear Schrödinger-type equation is thus considered as a linear equation within each iteration step and solved by means of methods from linear algebra supplying a orthonormal set of eigenfunctions and corresponding eigenvalues. The nonlinear behavior enters the procedure once again when the eigenfunctions are used to calculate for the next step the new mean-field potential the electron is moving in. After the fulfillment of some criteria of convergence for the iterations, the end product is a solution in terms of orthonormal wave functions, presumably representing the single-electron states of the problem.

In applications in quantum chemistry, it is often more appropriate to resort to functional basis that are not orthonormal in order to reduce the size of the numerical effort. A direct solution of the equations then leads to a general eigenvalue problem and solutions that are not orthonormal, but usually the orthonormality of the solutions is restored by a refined handling of the general eigenvalue problem \cite{4}.

For the fermion system (e.g. the electrons in a quantum dot), the hope is that the mean-field single-electron solutions that have been achieved by a self-consistent iteration of the Schrödinger equation and the equation for the mean-field potential reflects in some reasonable approximation properties of the original huge linear many-electron problem. Of course the individual single-electron states, wave functions, or orbitals are of limited value, but they can be used to construct more physically relevant entities like various response functions, the total energy, and the total charge distribution. Confidence in the method has come from comparison to numerical solutions of the corresponding truncated many-electron problem for few electrons \cite{5} \cite{6}, and experimental results.

For the boson system, namely, cold atoms in a trap, the ground state of the nonlinear GPE has been calculated in order to gain information about properties of the BEC, and the GPE has been generalized to finite temperatures by the means of self-consistent Hartree-Fock or Bogolyubov approximations where special care has been taken to construct orthonormal states for the system \cite{7}; otherwise, reasons are given for neglecting the fact that a particular approximation does not preserve the orthogonality \cite{8}.

After utilizing these methods for years in each of the mentioned subfields and comparing the different approaches, we would like to draw attention of the reader to interesting open questions concerning the nonlinearity of the underlying equations. In particular, we show that the nonlinear mean-field single-particle ground state is not a pure state where all boson particles would condense, like in standard linear quantum theory. It is a mixed state that allows a small part (less than one percent) of the boson gas to populate higher nonlinear excited energy levels. We present a simple model to highlight our concerns. We are of course aware that these mean-field equations do only asymptotically describe the respective systems within an appropriate range of physical parameters like many other celebrated equations in physics, even though they have been found to reproduce the properties of the systems outside of the parameter range that the approx-

\textsuperscript{1}Université de Nice - Sophia Antipolis, CNRS, Observatoire de la Côte d’Azur, BP 4229, 06304 - Nice Cédex 4, France
\textsuperscript{2}Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland

PACS numbers: 73.21.La 71.10.Li 71.90+q

I. INTRODUCTION

Commonly, quantum mechanical models of many interacting particles – linear models – are made computationally tractable by transforming them into a mean-field single-particle models, at the cost of making the model nonlinear, but solvable \cite{1}. Yet, solvable has a different meaning within two fields of condensed matter physics, the field of cold atoms in an external trap, and the field of electrons in a quantum dot. In the former field, the ensuing equation for the Bose-Einstein condensate (BEC), namely, the Gross-Pitaevskii equation (GPE), is often solved directly as a nonlinear differential equation \cite{2} \cite{3}. In the latter case, for electrons confined in a quantum dot, the approximation applied for the Coulomb interaction between the electrons leads to the Hartree, the Hartree-Fock, or Kohn-Sham type of an equation. All these are nonlinear equations that are conventionally solved by an iteration scheme. These equations for the electrons have a similar nonlinear term as for the GPE, but the long range nature of the Coulomb interaction makes them more complex. Within each iteration, the mean-field potential is constructed with information about the charge distribution and/or the wave functions from former iterations. The nonlinear Schrödinger-type equation is thus considered as a linear equation within each iteration step and solved by means of methods from linear algebra supplying a orthonormal set of eigenfunctions and corresponding eigenvalues. The nonlinear behavior enters the procedure once again when the eigenfunctions are used to calculate for the next step the new mean-field potential the electron is moving in. After the fulfillment of some criteria of convergence for the iterations, the end product is a solution in terms of orthonormal wave functions, presumably representing the single-electron states of the problem.

In applications in quantum chemistry, it is often more appropriate to resort to functional basis that are not orthonormal in order to reduce the size of the numerical effort. A direct solution of the equations then leads to a general eigenvalue problem and solutions that are not orthonormal, but usually the orthonormality of the solutions is restored by a refined handling of the general eigenvalue problem \cite{4}.

For the fermion system (e.g. the electrons in a quantum dot), the hope is that the mean-field single-electron solutions that have been achieved by a self-consistent iteration of the Schrödinger equation and the equation for the mean-field potential reflects in some reasonable approximation properties of the original huge linear many-electron problem. Of course the individual single-electron states, wave functions, or orbitals are of limited value, but they can be used to construct more physically relevant entities like various response functions, the total energy, and the total charge distribution. Confidence in the method has come from comparison to numerical solutions of the corresponding truncated many-electron problem for few electrons \cite{5} \cite{6}, and experimental results.

For the boson system, namely, cold atoms in a trap, the ground state of the nonlinear GPE has been calculated in order to gain information about properties of the BEC, and the GPE has been generalized to finite temperatures by the means of self-consistent Hartree-Fock or Bogolyubov approximations where special care has been taken to construct orthonormal states for the system \cite{7}; otherwise, reasons are given for neglecting the fact that a particular approximation does not preserve the orthogonality \cite{8}.

After utilizing these methods for years in each of the mentioned subfields and comparing the different approaches, we would like to draw attention of the reader to interesting open questions concerning the nonlinearity of the underlying equations. In particular, we show that the nonlinear mean-field single-particle ground state is not a pure state where all boson particles would condense, like in standard linear quantum theory. It is a mixed state that allows a small part (less than one percent) of the boson gas to populate higher nonlinear excited energy levels. We present a simple model to highlight our concerns. We are of course aware that these mean-field equations do only asymptotically describe the respective systems within an appropriate range of physical parameters like many other celebrated equations in physics, even though they have been found to reproduce the properties of the systems outside of the parameter range that the approx-
approach itself can be justified for. In the summary section we reflect on the physical relevance and interpretation of our findings.

II. THE NONLINEAR SCHRÖDINGER QUANTUM MODEL

Prior to the discovery of the microscopic BCS theory of superconductivity as a Bose condensation of electrons paired by microscopic electron-lattice interactions [9], tentative links of superconductivity with the interaction between electrons and lattice vibrations had already been explored [10] [11]. Most interesting in the scope of the present work is Schafroth’s early suggestion that charge-carrying bosons in a metal at low temperature actually constitute a gas of bound two-electron states [12] [13] which can then be described by a self-consistent normalized nonlinear Schrödinger-Poisson (SP) differential system [14]. At that time (1955), Schafroth just wanted to emphasize the role of long-range Coulomb interactions between bosons by use of mostly qualitative arguments. He assumed this charged boson gas to be defined by the stationary Schrödinger equation and proposed a one-dimensional (1D) SP model which considers the particles as moving in an effective potential \( V(x) \) related to Poisson’s equation to the local boson charge density with an additional uniform source term modeling both the charge density of the background (in order to make the whole system electrically neutral) and the non-condensed particles. Evidently, this uniform source term in 1D Poisson equation can be regarded as the second derivative of an additional external harmonic confining potential. Consequently, this 1954 SP model was probably the first model of a single, harmonically-trapped, stationary BEC with discrete non-orthogonal (since the equation is nonlinear) interfering eigenstates \( |\Psi_i\rangle \). Due to 2D radial axisymmetry, \( |\Psi_i\rangle = |\psi_i\rangle \otimes |m\rangle \) is an eigenstate of the angular-momentum operator with the eigenvalue \( mh \). As \( \langle \Psi_i|\Psi_j\rangle = \langle \psi_i|\psi_j\rangle \langle m_i|m_j\rangle \neq 0 \) only if \( m_i = m_j = 0 \), it is sufficient to consider the zero-angular-momentum states \( m = 0 \) in order to display peculiar physical properties related to Bose eigenstate non-orthogonality (in contrast with, e.g., BEC vortex-nucleation where the \( m = 1 \) nonlinear eigenstate, actually orthogonal to the \( m = 0 \) ground state, plays the major role [15]). The discrete radial one-particle Bose eigenfunction \( \psi_i(r) \) is defined in the mean-field approximation by the stationary Schrödinger equation related to the corresponding chemical-potential eigenvalue \( \mu_i \). In scaled form \( u_i(r) \propto \psi_i(r) \), it reads:

\[
\ddot{u}_i + \frac{1}{X} \dot{u}_i + \left[ \frac{\mu_i - \bar{\Phi}_i}{4} - \frac{X^2}{4} \right] u_i = 0,
\]

where the dot stands for derivation with respect to the radius \( X \) measured in units of the characteristic length \( l_0 = \sqrt{\hbar/2M\omega} \) and the tilde superscript labels energy in units of \( \hbar \omega \). The dimensionless particle-particle interaction energy \( \bar{\Phi}_i(r) \) per particle introduces into the system nonlinearity which is appropriately scaled to unity. Indeed, defining

\[
u_i(r) = \sqrt{\frac{\pi \hbar N_i}{M\omega}} \psi_i(r),
\]

where the dimensionless parameter \( N_i \) is self-consistently given by the solution of Eq. (1) according to

\[
\int_0^\infty u_i^2 X dX = N_i,
\]

we obtain the necessary 2D axisymmetric normalization condition

\[
\int |\Psi_i|^2 d^2x = \int \psi_i^2 2\pi r dr = 1,
\]

together with the scaling to unity of the nonlinear coefficient for both the GPE:

\[
\bar{\Phi}_i = u_i^2,
\]
and the SP differential system

\[ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \Phi_i - \frac{1}{s} \Phi_i = u_i^2. \tag{6} \]

Equation (6) defines the contact interactions of the hard-sphere BEC while the 2D Poisson Eq. (6) defines the long-range Coulomb interactions of the charged Bose gas (e.g., quantum-dot helium [6]). Practically, the value of the dimensionless norm \( s \) is given by the experimental conditions. We have \( N_1 = 4N(a_s/L_z) \) for the BEC defined by its scattering length \( a_s \) and extension \( L_z \) in the axial \( z \)-direction that contains \( N \) particles in the \( i \)th nonlinear eigenstate [13]. Specifically, \( N_1 \approx 30.29 \) for the ground state in Paris-ENS’ large laser-beam stirrer experiment [19, 21] while \( N_0 \approx 187.35 \) in Boulder-JILA’s rotating normal-cloud experiment [22, 23]. These high values \( N_1 \gg 1 \) of the nonlinear parameter are due to the number of atoms in the trap which is quite large (typically of order \( 10^{4-5} \)). They allow the ground state to be approximated by its localized “negative-curvature” parabolic Thomas-Fermi profile [2, 3] and define in the present work the so-called “classical-nonlinear” regime. On the other hand, the experimental parameters defining quantum-dot helium yields much lower values \( N_1 \approx 2 - 3 \) for the ground state nonlinearity [24], they would correspond in our study to the “quantum-nonlinear” regime where interference effects occur.

III. DISCUSSION

The interest in nonlinear quantum eigenstates can be illustrated for both the charged Bose gas defined by Eq. (6) and the GPE system defined by Eq. (5). In the former case, the nonlinear eigenstates can be regarded as unperturbed although they take into account, in addition to the particles’ external parabolic confinement, the (usually quite important) long-range Coulomb interactions [25]. In the later case, nonlinear quantum eigenstates in the physical description of very-many-particle stationary BEC’s are unavoidable. Indeed, there is practically no other choice than solving the nonlinear GPE (1) and (5). Therefore we numerically consider the discrete real-valued radial-symmetric normalized eigenstates \( u_i \) of Eqs. (1) and (5)-(6) which are by choice non-orthogonal since we restrict ourselves to \( m_i = 0 \) zero-angular-momentum \( s \) states [26]. Specifically, we consider the two first such eigenstates \( |u^1\rangle \) and \( |u^3\rangle \) whose superscript labels refer to their number of hard-core eigenquanta in the limit of vanishing nonlinearity, i.e., for the 2D linear parabolic system [6]. Their normalized inner product \( \langle u^1 | u^3 \rangle \neq 0 \) yields the statistical weight \( w^{13} = w^{31} = \langle |u^1|^2 |u^3|^2 \rangle = \langle |u^1|^2 \rangle \langle |u^3|^2 \rangle = 0 \) that defines the mixed ground state whose appropriate description in terms of the nonlinear density matrix \( \rho \) is

\[ \rho = \frac{1}{1 + w^{13}} |u^1\rangle \langle u^1| + \frac{w^{13}}{1 + w^{13}} |u^3\rangle \langle u^3|. \tag{7} \]

As a matter of fact, the standard use of a density matrix demands an orthonormal basis of eigenstates. Therefore, Eq. (7) should be understood as an extension of this concept to the nonlinear case where the eigenstates are not orthogonal. This generalization is all the more natural as the deviation from orthogonality is small (see below Fig. 1) and it yields a transparent physical interpretation. Indeed, Eq. (7) suggests that the probability per particle for the Bose gas to be in the nonlinear excited state \( |u^3\rangle \) is but its probability \( 1/(1 + w^{13}) \) to be in the nonlinear ground state \( |u^1\rangle \) multiplied by the mere transition probability \( w^{13} \) from \( |u^1\rangle \) to \( |u^3\rangle \). However this last expression must be taken in a somewhat loose sense since the present time-independent description is, strictly speaking, incompatible with the concept of a quantum transition (we will return to this discussion further below).

The paradoxical property, compared with standard linear theory, is that as the system is in the mixed state described by Eq. (7), it nevertheless allows interference between the two eigenstates \( |u^1\rangle \) and \( |u^3\rangle \) to occur, according to the following theorem:

\[ \langle u^1 | u^3 \rangle = \frac{\Phi^{1}_{31} + \Phi^{3}_{13}}{\mu_3 - \mu_1}. \tag{8} \]

The subscripts in \( \Phi^{i}_{jk} \) define the Hilbertian matrix elements of the particle-particle interaction potential \( \Phi^i \) corresponding to \( |u^i\rangle \) (see Eq. (1)). These elements have been calculated by use of the nonlinear eigenfunctions \( u^i \) while \( \mu_i \) are those nonlinear eigenvalues (or equivalently chemical potentials) which respectively define the \( u^i \)'s. Equation (7) is a direct consequence of the Hermiticity of the Laplacian operator in the Schrödinger equation (1) [27]. The first term on the r.h.s. of Eq. (8) defines the probability amplitude for the system in the nonlinear eigenstate \( |u^1\rangle \) to be also in the nonlinear eigenstate \( |u^3\rangle \), due to the interaction potential \( \Phi^1 \) defined by the probability density \( |u^1|^2 = (u^1)^2 \) through Eqs. (5) or (6), while the second term defines the reverse process, namely, the probability amplitude for the system in \( |u^3\rangle \) to be also in \( |u^1\rangle \) as a consequence of the interaction potential \( \Phi^3 \) defined by \( (u^3)^2 \). Equation (8) is exact. Therefore no perturbative-like ordering in \( \Phi^i \) is needed although, of course, a straightforward time-independent perturbation scheme that considers \( \Phi^i \) as perturbation in its respective Schrödinger equation (1) allows one to recover it (for instance when nonlinearity is weak). This point will be further developed in the next part.

The two amplitudes in Eq. (8) interfere because the corresponding \( 1 \leftrightarrow 3 \) processes are indistinguishable in the build-up of the probability amplitude \( \langle u^1 | u^3 \rangle \). Therefore this amplitude actually defines the nonlinear quantum coherence in our two-state system. The interference pattern is increased by the \( \omega \to 0 \) progressive flattening of the parabolic trap in the case of the confined charged Bose gas and by the increase of the particle number in the GPE system; or, equivalently for
both of them, by a progressive increase of the nonlinearity parameter $N$ in the system, as defined by Eq. [3].

Figure 1 illustrates in the case of 2D axisymmetric quantum dot helium the remarkable behavior of the normalized mixed-state statistical weight $w^{13} = (u^1|u^3)^2 = (u^1|u^3)^2$ where

$$\langle u^1|u^3 \rangle = \frac{1}{N} \int_0^\infty u^1 u^3 x dX.$$  \hspace{1cm} (9)

The two eigenstates $u^{1,3}$ must obviously correspond to the same physical system. For the GPE defined by Eq. [6], this means that their particle number should be the same and hence $N = N_1 = N_3$. The case of the confined charged Bose gas defined by Eq. [14] demands an additional condition which states that the external trap parabolicity $\omega$ is identical for both eigenstates $u_i$. Nevertheless it also yields $N = N_1 = N_3 = 14$. We numerically obtain the simple interference pattern

$$w^{13} = \gamma \sin^2 \left( \frac{N}{2} \right) + o(\gamma^2),$$  \hspace{1cm} (10)

for $N \leq 6$ and $\gamma = 2.29 \times 10^{-2}$. It displays a remarkable nonlinear resonance where the quantum coherence maximum is reached about the particular value $N = N^* \sim 3$. For quantum-dot helium, the only free physical parameter is the trap parabolicity $\omega$. Therefore we have $N \equiv N(\omega)$ and the resonance occurs for the particular parabolic trap profile $V(r) = \frac{1}{2} M \omega^2 r^2$ where $\omega^* = \omega(N^*)$. Numerical simulations in this 2D axisymmetric model show that $h\omega^* \sim 0.14 \epsilon$ where $\epsilon = Me^2/h^2$ is the effective atomic energy unit [24]. Hence $h\omega^* \sim 3.80$ eV for electrons in vacuum since $\epsilon = 27.21$ eV while $h\omega^* \sim 1.66$ meV in the case of GaAs quantum-dot helium where $\epsilon = 11.86$ meV.

In the case of long-range Coulomb particle-particle interactions described by Eq. [6], there exists a maximum amplitude $u_0$ for both nonlinear eigenstates $u^1$ and $u^3$ that is clearly visible on Fig. 2 when $N$ varies from $10^{-2}$ ($u_0 \sim 0.1$) to $10^2$ ($u_0 \sim 1$). For such high values of $N$, one reaches the classical asymptotic Thomas-Fermi regime defined by neglecting the quantum kinetic Laplacian derivative terms in Eq. [4] [14]. Then $\Phi(X) \sim \mu_i - X^2/4$ and Eq. [6] yield the common limit $u^1(X) \equiv u^3(X) \equiv u_{TF} \equiv 1$. The respective initial conditions of the two modes split.

FIG. 1: The quantum-dot helium interference pattern defined by the square probability amplitude $w^{13} = (u^1|u^3)^2$, as compared with its $\sin^2$ approximation defined by Eq. (10) (thin continuous line). There occurs a clearly visible threshold at $N \sim 6$ where the system bifurcates from its interfering quantum regime towards its Thomas-Fermi classical one.

FIG. 2: The convergence in the $\{ C_0 = \tilde{\mu} - \Phi(0) \}$ vs $\{ u_0 = u(0) \}$ initial-condition phase space of the two-level SP nonlinear system defined by $u^1$ (lower red curve) and $u^3$ (upper blue curve) towards the common fixed point $u_0 = 1$ and $C_0 = 0$ when the nonlinearity parameter increases from the linear regime $N \sim 10^{-2}$ to the classical Thomas-Fermi one defined by $N \sim 10^2$. The corresponding common asymptotic eigenstate profile $u_{TF}(X)$ for these two first $m = 0$ nonlinear eigenmodes is the uniform one $u_{TF} \equiv 1$.

FIG. 3: The convergence of the GPE system (5) towards the THF classical regime still defined by $\Phi(X) \sim \mu_i - X^2/4$, as shown by Fig. 4. Then we indeed have $\lim_{N \to \infty} C_0 = \lim_{N \to \infty} (\tilde{\mu} - \Phi(0)) = \lim_{N \to \infty} (\mu_i - u_0) = 0$, but the nonlinear eigenstate amplitudes $u_0$ grow without limit while their corresponding profiles converge towards $u_{TF}(X) \equiv \sqrt{\mu_i - X^2/4}$, as shown by Eqs. 4 and 5 when the Laplacian derivative terms are neglected. There is no bifurcation from the amplitude-growing regime to the width-growing one, like in the SP case displayed by Figs. 2 and 3. It can be said that, due to GPE particle-particle contact interactions defined by Eq. (5), the bosons pile up in the trap rather
FIG. 3: The nonlinear SP eigenstate profiles $u^1$ (continuous) and $u^3$ (dashed) for increasing values $N \leq 8$ of the nonlinearity. Note the last $u^1$ and $u^3$ profiles where the width—instead of the amplitude—starts increasing.

FIG. 4: The convergence in the $\{C_0 = \tilde{\mu} - \tilde{\Phi}(0) = \tilde{\mu} - u_0^2 \}$ vs $\{u_0 = u(0)\}$ initial-condition phase space of the three-level GPE system defined by its $m = 0$ nonlinear states $u^1$ (lower blue curve), $u^3$ (middle pink curve) and $u^5$ (upper red curve) towards the common fixed point $u_0 = \infty$ and $C_0 = 0$ when the nonlinearity parameter increases from the linear regime $N \sim 10^{-2}$ towards the classical Thomas-Fermi one $N \gg 1$. The corresponding common asymptotic eigenstate profile $u_{TF}(X)$ for these nonlinear eigenmodes is defined by $u_{TF} \equiv \sqrt{\tilde{\mu} - X^2/4}$ as shown by Eqs. (4) and (5) when the Laplacian derivative terms are neglected.

FIG. 5: The interference pattern defined by the square probability amplitude $w^{ij} = \langle u^i | u^j \rangle^2$ in the case of the GPE system. The threshold for the quantum-classical transition occurs at $N \sim 10$.

IV. CONCLUSION

The nonlinear eigenstates $|i\rangle$ that have been defined and discussed in the present work are time-independent. Since the nonlinear term in Eq. (1) is a (square) modulus in the corresponding time-dependent Schrödinger equation, its eigenstates $\Psi^i \propto u^i e^{i\mu^i t/\hbar}$ do still have the standard time dependence related to the eigenvalue $\mu^i$ of $|i\rangle$. A conceptual problem arises when one considers the interaction between such states. Indeed, due to their non-orthogonality defined by Eq. (9) and illustrated by Figs. 1 and 5, one cannot state any more that the system is in the pure stationary eigenstate $|i\rangle$. It has the probability amplitude $(j|i)$ defined by Eq. (8) to be also in some other nonlinear state $|j\rangle$. The statistical weight $w^{ij} = (j|i)^2$ then defines the corresponding mixed state in accordance with Eq. (7). Actually $w^{ij}$ is quite small: typically less than 1% (cf. Eq. (10)). This might explain the quite acceptable results obtained in GPE systems when one neglects $w^{ij}$ and assumes that all the boson particles have condensed in the ground state. Nevertheless, this statement is formally wrong and might yield a weak measurable departure from the expected GPE ground state particle density in accurate BEC experiments.

It is tempting to relate $w^{ij}$ to a mere transition probability. Again, the result is unexpected. Indeed, assume that the nonlinearity $N = N_i = N_j$ is small. Therefore each interaction potential $\tilde{\Phi}^{i,j}$ may be regarded as a perturbation in its corresponding Schrödinger equation (1). Using standard time-independent perturbation theory, one obtains $\Phi_{ij}^{ij}/(E_i - E_j)$ (resp. $\Phi_{ji}^{ji}/(E_j - E_i)$) as the probability amplitude for the system being in $i$th (resp. $j$th) linear eigenstate of energy $E_i$ (resp. $E_j$) to be also in the $j$th (resp. $i$th) linear eigenstate of energy $E_j$ (resp. $E_i$). One recognizes in the two terms of Eq. (8) the simple extrapolation of these probability amplitudes to any value of the perturbation (i.e. of the nonlinearity) while the linear energy eigenvalues $E_{i,j}$ become the corresponding (nonlinear) chemical-potential $\mu_{i,j}$. However, due to
nonlinear quantum coherence, there is no simple relationship between each such probability amplitude and a possible transition probability. Indeed, for the \(\{|i\}, \{|j\}\) two-state system, exact diagonalization of the perturbed Hamiltonian in the time-dependent Schrödinger equation is possible. It yields in first-order with respect to \(\Phi\) the so-called Fermi golden rule transition probability \(\langle i \rightarrow j \rangle\)

\[
P_{i \rightarrow j} = 4 \left[ \frac{\Phi_{ji}}{E_i - E_j} \right]^2 \sin^2 \left( \frac{E_i - E_j}{2\hbar} t \right) + o(\Phi^3) \quad (11)
\]
or reverse [25]. Since Eq. (11) is exact, one can average it for \(t \gg \hbar/(E_i - E_j)\) and obtain \(P_{i \rightarrow j} \sim 2 \left[ \frac{\langle \Phi_{ji} \rangle}{(E_i - E_j)} \right]^2\) in the lowest order in \(\Phi^2\); which, apart from the factor 2, is indeed the square time-independent probability amplitude that has been previously obtained. However, to Eq. (5), the statistical weight \(w^{ij} = \langle j|i \rangle^2\) is not merely equal to the extrapolation of \(P = \frac{1}{2}(P_{i \rightarrow j} + P_{j \rightarrow i})\) to any value of the nonlinearity parameter \(\lambda\). There remains twice the probability amplitude product which lowers \(P\) by more than one order of magnitude.

By focusing our attention on the nonlinear character of two simple cases, the present paper actually aims to be introductory in the field concerning the reduction of the original 3N-dimensional ground-state wave vector defining a N-particle linear quantum system to the 3D one-particle mean-field nonlinear Schrödinger description based on the mixed ground state given by Eq. (7). The conclusion that the nonlinear Schrödinger equation, like many other similar ones, is only intended as a recipe to obtain a solution within an iteration scheme where the problem is considered linear at each iteration step lies close at hand. However, it remains an open question whether the direct solution of the nonlinear problem yields properties that are not obtainable in the iteration scheme, and indeed, if such inherent nonlinear properties have a physical relevance. While the (mostly numerical) investigations of the time-dependent GPE mainly concern linear surface excitations of the condensate about its stationary asymptotic ThF ground state profile, true time-dependent nonlinear structures such as the breathing monopole oscillation mode have been pointed out [2]. These structures are actually solitons, like in the case of two-BEC time-dependent interferences [17]. We recall that solitons provide a paradigm example of a true nonlinear phenomenon that can never be described as a convergent limit of a linear iterative process. Such seems also the case for the quantum properties related to non-orthogonality between the one-particle mean-field nonlinear eigenstates. Therefore, any attempt to investigate the time-dependent relationship between linear and nonlinear eigenstates of a given quantum system — like the recent attempt to both display particular nonlinear eigenfunctions as global attractors for all finite-energy solutions and describe quantum transitions between them [28]— are welcome. However, only a comparison with experiments and the solutions of the original linear many-particle problem can shed a definite light on these questions.

Acknowledgments

The authors acknowledge financial support from the Icelandic Research and Instruments Funds, the Research Fund of the University of Iceland and the University of Nice (France).

[1] W. Kohn, Rev. Mod. Phys. 71, 1253 (1998).
[2] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 71, 463 (1999).
[3] A. J. Leggett, Rev. Mod. Phys. 73, 307 (2001).
[4] V. Luaña, A. O. de la Roza, M. A. Blanco, and J. M. Recio, European Journal of Physics 31, 101 (2010).
[5] P. A. Maksym and T. Chakraborty, Phys. Rev. Lett 65, 108 (1990).
[6] D. Pfannkuche, V. Gudmundsson, and P. Maksym, Phys. Rev. E 47, 2244 (1993).
[7] D. A. Huse and E. D. Siggia, Journal of Low Temperature Physics 46, 137 (1982).
[8] V. V. Goldman, I. F. Silvera, and A. J. Leggett, Phys. Rev. B 24, 2870 (1981).
[9] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. 106, 162 (1957).
[10] H. Fröhlich, Phys. Rev. 79, 845 (1950).
[11] J. Bardeen, J. Mod. Phys. 23, 261 (1951).
[12] M. R. Schafroth, Phys. Rev. 96, 1442 (1954).
[13] M. R. Schafroth, Phys. Rev. 96, 1149 (1954).
[14] M. R. Schafroth, Phys. Rev. 100, 463 (1955).
[15] L. L. Foldy, Phys. Rev. 124, 649 (1961).
[16] A. S. Alexandrov and W. H. Beere, Phys. Rev. B 51, 5887 (1995).
[17] W.-M. Liu, B. Wu, and Q. Niu, Phys. Rev. Letters 84, 2294 (2000).
[18] G. Reinisch, Phys. Rev. Lett. 99, 120402 (2007).
[19] K. W. Madison, F. Chevy, W. Wohlleben, and J. Dalibard, Phys. Rev. Lett. 84, 806 (2000).
[20] F. Chevy, K. W. Madison, and J. Dalibard, Phys. Rev. Lett. 85, 2223 (2000).
[21] K. W. Madison, F. Chevy, V. Bretin, and J. Dalibard, Phys. Rev. Lett. 86, 4443 (2001).
[22] M. R. Matthews, B. P. Anderson, P. C. Haljan, D. S. Hall, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. 83, 2498 (1999).
[23] P. C. Haljan, I. Coddington, P. Engels, and E. A. Cornell, Phys. Rev. Lett. 87, 210403 (2001).
[24] G. Reinisch and V. Gudmundsson, arXiv:0906.4650 (2009), URL http://arxiv.org/abs/0906.4650
[25] C. Cohen-Tannoudji, J. Dupont-Roc, and G. Gryndberg, Processus d’interaction entre photons et atomes (InterEditions, Editions du CNRS (Paris), 1988).
[26] G. Reinisch, Phys. Rev. A 70, 033613 (2004).
[27] J. Bec, private communication (2010).
[28] A. Komech and A. Komech, arXiv:math/0609013 (2006), URL http://arxiv.org/abs/math/0609013.