The Quantum Josephson Hamiltonian In The Phase Representation

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(March 21, 2022)

Abstract

The quantum Josephson Hamiltonian of two weakly linked Bose-Einstein condensates is written in an overcomplete phase representation, thus avoiding the problem of defining a Hermitian phase operator. We discuss the limit of validity of the standard, non-rigorous Mathieu equation, due to the onset of a higher order \( \cos 2\phi \) term in the Josephson potential, and also to the overcompleteness of the representation (the phase \( \phi \) being the relative phase between the two condensates). We thereby unify the Boson Hubbard and Quantum Phase models.

PACS: 74.50.+r,03.75.Fi
Recent developments on the engineering of Bose-Einstein condensates (BEC’s) [1,2] are suggesting new scenarios for searching macroscopic quantum coherence phenomena. Most of the dynamical regimes investigated experimentally have been understood within the Gross-Pitaevskii (GP) framework [3]. GP is essentially a “classical” theory, since it approximates the quantum bosonic field as a complex order parameter [4]: the new challenge is the systematic study of regimes where quantum fluctuations cannot be ignored.

Quantum effects play an important role in a “mesoscopic” Josephson junction [5]. The Josephson effects (JE) are a paradigm of phase coherence in superfluid/superconductive systems [3,4]. In the BEC context, JE have been associated with coherent collective oscillations between two weakly-linked condensates, the weak link being created by the potential barrier in a double-well trap [7,8], or by a quasi-resonant external electromagnetic field, which induces oscillations between two trapping hyperfine levels [4,5]. Although bosons are neutral, and external circuits are obviously absent, it is also possible to study the close analogs of the the “ac” and “dc” effects observed in superconducting Josephson junctions [10]. Quite recently, an array of “mesoscopic” weakly linked condensates has been created in [9], each trap, located at the antinodes of an optical standing wave, containing \( \sim 1000 \) condensate atoms.

The classical Josephson Hamiltonian (CJH) has been casted in term of a pendulum-like equation [7,17]:

\[
H_{cl} = \frac{E_c}{2} n^2 - \frac{2E_J}{N} \sqrt{N^2/4 - n^2} \cos \phi
\]

with the relative number of condensate atoms between the two bulk condensate \( n = \frac{1}{2}(n_1 - n_2) \) playing the role of the momentum, and the relative phase \( \phi = \phi_1 - \phi_2 \) being the angle respect to the horizontal axis [18].

The “charging energy” \( E_c \) and the “Josephson coupling energy” \( E_J \) can be calculated as overlap integrals [7,10]:

\[
E_c = 2g \int dr \Phi_1(r)^4 = 2g \int dr \Phi_2(r)^4
\]  

(2a)
\[
E_J = -N \int dr \, \Phi_1(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}} + \frac{gN}{2} [\Phi_1^2(r) + \Phi_2^2(r)] \right] \Phi_2(r) \tag{2b}
\]

with the one-body wave functions \( \Phi_1(r), \Phi_2(r) \) localized in the trap 1, 2, respectively, and \( f dr \, \Phi_1(r)^* \Phi_2(r) = 0 \), \( f dr \, |\Phi_{1,2}(r)| = 1 \), \( g = \frac{4\pi\hbar a}{m} \); \( a \) being the scattering length and \( m \) the atomic mass; \( N \) is the total number of atoms \[13\].

The quantum Josephson Hamiltonian (QJH), on the other hand, has been studied within two different models which seem in conflict with each other \[20\]. This conflict originates, at its heart, from a fundamental, yet unsolved, problem: the existence and the meaning of a quantum phase operator \[21\].

In the “boson mode” representation, QJH is written in terms of creation and destruction boson operators \[1,12,13,15\]:

\[
\hat{H} = \frac{E_c}{4} (\hat{a}_1^+ \hat{a}_1 \hat{a}_2 \hat{a}_2 + \hat{a}_2^+ \hat{a}_2 \hat{a}_1 \hat{a}_1) - \frac{E_J}{N} (\hat{a}_1^+ \hat{a}_2 + \hat{a}_2^+ \hat{a}_1) \tag{3}
\]

where \( \hat{a}_{1,2}, (\hat{a}_{1,2}) \) creates (destroys) a particle in the trap 1, 2, respectively.

In the “phase” representation, on the other hand, the relevant quantum observables are the difference of phases and number of atoms between the two condensates in each trap \[11,22,23\], the Hamiltonian being written in term of a “quantum pendulum” (Mathieu) equation:

\[
\hat{H} = -\frac{E_c}{2} \frac{\partial^2}{\partial \phi^2} - E_J \cos \phi \tag{4}
\]

with \( \hat{n}^2 = (\hat{a}_1^+ \hat{a}_1 - \hat{a}_2^+ \hat{a}_2)^2 \sim -\frac{\partial^2}{\partial \phi^2} \) and \( \hat{\phi} \) which cannot, as we will discuss shortly, be unambiguously defined in terms of creation/destruction operators. Eq. (4) acts on a \( 2\pi \)-periodic “wave-function” \( \psi(\phi) = \psi(\phi + 2\pi) \), with \( \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi \, \psi(\phi)^* \psi(\phi) = 1 \) and expectation values \( \langle \hat{A} \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi \, \psi(\phi)^* A(\phi, t) \psi(\phi) \). This framework, generalized to include damping effects and external circuits, is rather standard in the SJJ literature \[23\].

Generally speaking, the Hamiltonian Eq. (3) can be derived microscopically from the quantum field equation:

\[
\hat{H} = \int dr \, \hat{\Psi}^+ \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}} + \frac{g}{2} \hat{\Psi}^+ \hat{\Psi} \right] \hat{\Psi} \tag{5}
\]
writing the boson field in the “two-mode approximation” as: 
\[ \hat{\Psi} \simeq \Phi_1(r) \hat{a}_1 + \Phi_2(r) \hat{a}_2. \]

The quantum pendulum Eq. (4), on the other hand, can be retrieved quantizing the classical Josephson Hamiltonian Eq. (1) by replacing the classically conjugate phase/atom number with the corresponding, non-commuting, operators [29].

On this grounds we can consider Eq. (4) as a phenomenological, while Eq. (3) has a clearer “microscopical” foundation: it is generally believed that, for some limit, these two Josephson Hamiltonians describe essentially the same physics, yet, their exact relation has not been exploited in the literature. A way to analyze, a posteriori, the relation between the two Hamiltonians Eq. (3) and Eq. (4), is to identify:

\[ \hat{a}_i \equiv e^{i\hat{\phi}_i} \hat{n}_i^{1/2} \]  

with \( \hat{\phi}_i \) and \( \hat{n}_i = \hat{a}_i^+ \hat{a}_i \) Hermitian phase and number operators acting in the trap \( i \). The assumed Hermiticity of \( \hat{\phi}_i \) implies the unitarity of \( \exp(i\hat{\phi}_i) \). Number and phase, thus, are treated as conjugate observables:

\[ [\hat{\phi}_i, \hat{n}_i] = i \]  

which implies, in the phase-representation, \( \hat{n}_i \equiv -i\frac{\partial}{\partial \hat{\phi}_i}, \hat{\phi}_i \equiv \phi_i \). This approach is known to be incorrect. The commutator gives rise to inconsistencies when its matrix elements are calculated in a number-state basis. Even worse, the exponential operator \( \exp(i\hat{\phi}) \) is not unitary and so does not define an Hermitian \( \hat{\phi} \) [21].

Despite such problems, the Josephson Hamiltonian, Eq. (4), is considered as the starting point of most analysis in SJJ and BJJ, the implicit caveat being that the commutator relation Eq. (7) is approximately correct for systems with a large number of “condensate” Cooper-pairs/atoms. More precisely, the relation between Eq. (3) and Eq. (4) is considered only in a semiclassical context, replacing \( \hat{a}_{1,2} \rightarrow n_{1,2} e^{i\phi_{1,2}}, \) \( n_{1,2} \) being \( c \)-numbers, in the term proportional to the Josephson coupling energy \( E_J \) in Eq. (4).

In this letter we develops a consistent procedure to rewrite the quantum Josephson Hamiltonian Eq. (3) in the phase representation, overcoming the problem of defining an
Hermitian phase operator. The resulting equation differs in several ways from the Mathieu equation Eq. (4), which is recovered in a specific limit. Although we consider, for simplicity, the case of a two-sites Josephson junction, our analysis clarifies the relation between the Boson Hubbard [24,25] (which can be seen as the $n$-sites generalization of Eq. (3)) and the Quantum Phase models ($n$-sites generalization of Eq. (4)) [26], governing the dynamics of a BEC’s array as that created in [1].

An arbitrary state spanning the two-dimensional Hilbert space, in which is defined the QJH Eq. (3), can be expanded as:

$$|\psi\rangle = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} d\phi_1 d\phi_2 \ f(\phi_1, \phi_2) |\phi_1, \phi_2\rangle$$

(8)

with the (un-normalized) Bargmann state [27]:

$$|\phi_1, \phi_2\rangle = \sum_{l,m=0}^{\infty} e^{i(l\phi_1 + m\phi_2)} \frac{1}{\sqrt{l!m!}} |l\rangle |m\rangle$$

(9)

with $|m\rangle, |l\rangle$ atom number eigenstates of trap 1, 2 respectively.

In the Bargmann space, the action of the boson operators on the state vector Eq. (8) reduces to differential operators acting on $f(\phi_1, \phi_2)$:

$$f(\phi_i) \hat{a}_i \rightarrow e^{i\phi_i} f(\phi_i)$$

(10a)

$$f(\phi_i) \hat{a}_i^+ \rightarrow i \frac{\partial}{\partial \phi_i} \left[ e^{-i\phi_i} f(\phi_i) \right]$$

(10b)

as can be seen after an integration by parts. In particular, the atom number operator assumes the familiar form: $f(\phi_i) \hat{n}_i = f(\phi_i) \hat{a}_i^+ \hat{a}_i \rightarrow -i \frac{\partial}{\partial \phi_i} f(\phi_i)$.

We consider as fixed the total number of atoms, and we can write:

$$f(\phi, \phi_+) = e^{-iN\phi} \psi(\phi)$$

(11)

with $\phi_+ = \frac{1}{2}(\phi_1 + \phi_2)$, $\phi = \phi_1 - \phi_2$, $N = n_1 + n_2$, $n = \frac{1}{2}(n_1 - n_2)$, $N$ and $n$ being the total and the relative number of atoms. $\psi(\phi)$ is an arbitrary, $2\pi$-periodic function normalized to unity: $\frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi |\psi(\phi)|^2 = 1$. We can integrate over $\phi_+$ the Eq. (8):

$$|\psi\rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi \ \psi(\phi) |\phi\rangle$$

(12)
that can be considered, in the large $N$ limit, as a pure phase state $[22]$. The state Eq. (13) is proportional (with $\phi = 0$) to the exact ground state of Eq. (3) in the non-interacting limit ($E_c = 0$). Here we consider the states $|\phi\rangle$ as an overcomplete base to expand the solution of the full Josephson Hamiltonian Eq. (3). The scalar product of two phase states is given by:

$$
\langle \psi | \psi \rangle = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} d\theta \int_{-\pi}^{\pi} d\phi \, \psi(\theta)^* \psi(\phi) \langle \theta | \phi \rangle = 1 \tag{14a}
$$

$$
\langle \theta | \phi \rangle = \frac{N}{2} \sum_{n=-N/2}^{N/2} \frac{e^{in(\phi-\theta)}}{(\frac{N}{2}+n)! \left(\frac{N}{2}-n\right)!} = \frac{2^N N^2}{N!} \cos^N \left(\frac{\theta - \phi}{2}\right) = \frac{2^N}{(N!)^2} \delta_N(\phi - \theta) \tag{14b}
$$

In the limit of large number of atoms, $\langle \theta | \phi \rangle$ becomes proportional (in the interval $-\pi \leq \phi, \theta < \pi$) to a delta function:

$$
\lim_{N \to \infty} \delta_N(\phi - \theta) = \delta(\phi - \theta) \tag{15}
$$

The action of the Josephson Hamiltonian Eq. (3) on the state vector Eq. (12) gives:

$$
\hat{H} |\psi\rangle = (\hat{H}_c + \hat{H}_J) |\psi\rangle \tag{16a}
$$

$$
\hat{H}_c |\psi\rangle = \frac{E_c}{4} \int_{-\pi}^{\pi} d\phi \, |\phi\rangle \left[ -2 \frac{\partial^2}{\partial \phi^2} + \left( \frac{1}{2} N^2 - N \right) \right] \psi(\phi) \tag{16b}
$$

$$
\hat{H}_J |\psi\rangle = -\frac{E_J}{N} \int_{-\pi}^{\pi} d\phi \, |\phi\rangle \left[ (N + 2) \cos \phi + 2 \sin \phi \frac{\partial}{\partial \phi} \right] \psi(\phi) \tag{16c}
$$

Projecting out in the phase space:

$$
\langle \theta | \hat{H} |\psi\rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi \, \hat{F} \, \psi(\phi) \langle \theta | \phi \rangle \tag{17a}
$$

$$
\hat{F} \, \psi(\phi) \equiv \left[ -\frac{E_c}{2} \frac{\partial^2}{\partial \phi^2} - E_J \left( 1 + \frac{2}{N} \right) \cos \phi - \frac{2 E_J}{N} \sin \phi \frac{\partial}{\partial \phi} \right] \psi(\phi) \tag{17b}
$$

where a constant energy shift has been omitted. The spectrum of $\hat{H}$ is given by the eigenvalue equation for this $\hat{F}$, which is known as the Ince equation $[28]$. Notice that, because of the
overcompleteness of the phase-states Eq. (13), \( \hat{H}_J \) in Eq. (16(c) is Hermitian, even though the differential operator \( \sin \phi \frac{\partial}{\partial \phi} \) is not.

Thus the time-dependent Schrödinger equation in our phase representation,

\[
i \frac{\partial}{\partial t} \langle \phi | \psi \rangle - \langle \phi | (\hat{H}_c + \hat{H}_J) | \psi \rangle = 0 ,
\]

(18)
can be put in dimensionless form (by defining \( \gamma = \frac{2E_J}{E_c} \frac{1}{N} \) and rescaling \( t \rightarrow t \frac{E_c}{2} \)) as

\[
\int_{-\pi}^{\pi} d\phi \delta_N(\phi - \theta) \left[ i \frac{\partial}{\partial t} + \frac{\partial^2}{\partial \phi^2} + \gamma(N + 2) \cos \phi + 2\gamma \sin \phi \frac{\partial}{\partial \phi} \right] \psi(\phi) = 0 \tag{19}
\]

We may obtain a more transparent form of (19) by defining \( \psi(\phi) = e^{\gamma \cos \phi} \Psi(\phi) \). This eliminates the first derivative and, dropping a constant, maps \( \hat{F} \) onto a manifestly Hermitian operator acting on \( \Psi \). The result is that to satisfy Eq. (19) it is sufficient to satisfy

\[
i \frac{\partial \Psi}{\partial t} = \left[ -\frac{\partial^2}{\partial \phi^2} - \gamma(N + 1) \cos \phi - \frac{1}{2} \gamma^2 \cos 2\phi \right] \Psi \tag{20}
\]

Setting \( i \frac{\partial \Psi}{\partial t} = E \Psi \) gives the three-term Hill equation [28].

Eq. (20) is of the same usefully simple form as the QPM. One can apply to it all the intuition and experience, and all the calculational tools, that are relevant to the one-particle Schrödinger equation with a periodic potential. Solving it yields the energy spectrum of the BHM, and thus any dynamical time scales (such as for decay of the possible metastable states by tunneling). But since the equation is based on an overcomplete representation, expectation values and matrix elements must be computed using the nonstandard inner product with the kernel \( \delta_N \), and with the extra \( e^{\gamma \cos \phi} \) factors; hence the interpretation of the eigenstates can be somewhat subtle. Since \( \delta_N \), with \( N \gg 1 \), behaves as a delta function for test functions varying slowly on the scale \( N^{-1/2} \), for the lower energy states the inner product is essentially the standard one, and Eq. (20) can be used without any extra thought. For the higher energy states, however, the interpretations of \( \Psi(\phi) \) and Eq. (20) depend on \( \gamma \).

We can distinguish three regimes. For \( \gamma \geq \mathcal{O}(N) \), the \( \cos 2\phi \) term in (20) is a significant correction to the purely \( \cos \phi \) potential of the QPM; and for \( \gamma > N/2 \) it makes a second local
minimum at $\phi = \pi$. This agrees with the GPE result that for $\gamma > N/2$ there are metastable $\pi$-oscillations of zero average $n$. But the trapping of probability near $\phi = \pi$ is not trivial, because $e^{\gamma \cos \phi}$ factor tends strongly to suppress it. This suppression is countered for high energy states, however, by the fact that $\delta_N$ effectively eliminates all Fourier components $e^{ik\phi}$ with $|k| > N/2$ in $\psi(\phi)$. (This is as it should be, since from our derivation it is clear that such components are unphysical.) There are thus high energy solutions to Eq. (20) whose physical components are localized around $\phi = \pi$, because in the deeper well around $\phi = 0$ their WKB frequency has $|k| > N/2$. In the intermediate range of energies, however, the implications of $\delta_N$ are more complicated. Eqn. (20) may still be treated with semiclassical methods, as will be discussed elsewhere. It is qualitatively clear that both the second minimum of the potential, and the failure of quantum motion to be strictly confined to it, will be important; and so we must consider (20) as giving corrections to both the QPM and the GPE.

For $1 < \gamma << N$, the $\cos 2\phi$ term is insignificant, and so the eigenfunctions of Eq. (20) are essentially the Mathieu functions of the QPM. The nonlocality of $\delta_N$ is of little qualitative significance, except for the highest energy states. These are well approximated by the WKB method, and their local wave number is of the form $k + \gamma \frac{N+1}{2k} \cos \phi$. For $k$ of order $N/2$, this implies that solutions to (20) of the ‘running’ type, with no localized phase, actually have their physical component localized around $\phi = \pi$. This supports the GPE in what is its only significant discrepancy with the QPM in this range of $\gamma$, for the GPE also predicts high energy $\pi$-states with nonzero average $n$ [7]. (We neglect the fact that the actual quantum eigenstates must have zero average $n$, because they are even and odd ‘Schrödinger’s Cat’ superpositions of the states with large positive and negative $n$. But the splitting is exponentially small in $N$.)

For $\gamma \leq 1$, the situation is similar, except that the modulation of the local wave number with $\phi$ is too small for the elimination of unphysical Fourier components to produce a localized state. It simply eliminates all WKB states with $|k| > N/2$, and the result is that the physical spectrum of Eq. (20) is essentially Mathieu functions, up to a cut-off. The $\pi$-states of the GPE are absent and the QPM is vindicated, except for the welcome truncation
of the spectrum, in accordance with the fact that the Hilbert space must indeed be only $(N + 1)$-dimensional.

In Fig. (1) we draw the probability in phase, $P(\phi)$, in an orthonormal representation of $\phi$. This illustrates the interpretation of our nonorthonormal phase representation with unphysical components projected out. Considering $N = 199$ particles and $\gamma = N/5$, all 200 energy eigenstates are found numerically in the number basis, and ranked in order of energy. The absolute square of the Fourier transform of the number amplitudes is plotted for each state; since all $P(\phi)$ are even, only $0 \leq \phi \leq \pi$ is shown. This approach is not possible for large $N$, but it illustrates and confirms our discussion of the physical interpretation of our overcomplete representation, which is useful for all $N$. For this value of $\gamma$, Josephson-localized, running, and $\pi$-localized states all occur.

To conclude, a few words are in order about the Rabi limit $\gamma \to \infty$. In this case the potential of Eq. (20) becomes a pair of strong harmonic potentials centred at $\phi = 0$ and $\phi = \pi$, both having the frequency $\gamma E_c = 2E_J/N$. The equally spaced harmonic oscillator eigenstates of these potentials, up to the cut-off described earlier, reproduce the Rabi spectrum of the Hamiltonian (3) in the limit $E_c \to 0$.

This work has been partially supported by the Cofinanziamento MURST.
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[17] Here and in the following we consider a BEC in a symmetric double-well potential. In the case of an asymmetric potential we should add a term proportional to $n$ that is irrelevant for our present purposes. Terms proportional to $\int dr \, \Phi_1(r)^2 \, \Phi_2(r)^2$ are also neglected.

[18] Peculiar is the “non-rigidity” of the pendulum, which has a momentum dependent length $\sim \sqrt{N^2/4 - n^2}$. This allows stable pendulum oscillations about the up-right position, i.e. $\pi$-oscillations.

[19] It is clear, in this context, that the Josephson Hamiltonian Eq. (1) is “classical” in the sense that it considers the conjugate relative phase $\phi$ and number of atoms $n$ as c-numbers.

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[29] However this formal replacement can be pursued only in the limit $n \ll N; E_c \gg E_J/N^2$ so to keep only the zero-order expansion term of the square-root in Eq. (I).
FIGURES

FIG. 1. The module square of the energy eigenstates $P(\phi)$, as a function of an orthonormal representation of $\phi$, with $N = 199$ and $\gamma = N/5$. 
$P(\phi)$