

## Exact quantum phase model for mesoscopic Josephson junctions

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Starting from the two-mode Bose-Hubbard model, we derive an exact version of the standard Mathieu equation governing the wave function of a Josephson junction. For a finite number of particles  $N$ , we find an additional  $\cos 2\phi$  term in the potential. We also find that the inner product in this representation is nonlocal in  $\phi$ . Our model exhibits phenomena, such as  $\pi$  oscillations, which are not found in the standard phase model, but have been predicted from Gross-Pitaevskii mean-field theory.

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Exploring the quantum classical frontier is a major unifying theme of contemporary physics. An established check-point on this frontier is the Josephson junction (JJ), where in the limit of a very large number of particles  $N$ , the quantum phase difference  $\phi$  becomes an effectively classical degree of freedom. Recent experiments [1] have approached the mesoscopic regime of intermediate  $N$ , in which  $\phi$  may possibly be classical enough to manipulate, but quantal enough to exploit for such technologies as quantum computation [2]. Similar experiments have been proposed using trapped dilute Bose-Einstein condensates, in which  $N \sim 10^3 - 10^5$ ; and the manipulation of phase fluctuations in an array of weakly coupled Bose-Einstein condensates has been reported in [3]. The standard quantum theory of a JJ is the quantum phase model (QPM) [5], which treats  $\phi$  as a quantum-mechanical coordinate with a periodic potential. As well as explaining basic results, this theory is tractable enough to guide work on more complex problems (e.g., quantum computation in [2], phase cooling in [4]); but it is only derived for large  $N$ . In this paper, we provide an exact quantum phase model (EQPM), valid for all  $N$ . We thus extend the applicability of a useful quantum theory into the mesoscopic regime. We also provide a quantum-mechanical theory for mesoscopic phenomena that have previously been predicted semiclassically using the Gross-Pitaevskii mean-field theory (MFT)—another widely used theory [6] whose ratio of tractability to accuracy makes it extremely useful, and whose applicability in the mesoscopic regime needs more investigation. Josephson oscillations about  $\phi = \pi$ , which do not appear in the QPM, have been predicted from MFT [7], and compared [8] with those recently observed in <sup>3</sup>He [9]. Our exact and fully quantum-mechanical EQPM may exhibit these  $\pi$  oscillations in a wide regime.

Our derivation begins with the idealization of a mesoscopic JJ as a two-mode bosonic system. Generalizations to incorporate more modes may obviously be required for some realistic scenarios, but such generalizations may be made straightforwardly (if perhaps laboriously), and we will restrict ourselves to two modes for illustration. (Regimes in

which the two-mode model is actually an accurate approximation, to describe condensates in double-well traps, or two-component condensates, have recently been discussed [10–15].) We assume the Hamiltonian

$$\hat{H} = \frac{E_c}{4} (\hat{a}_1^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_2) - \frac{E_J}{N} (\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1), \quad (1)$$

where  $\hat{a}_{1,2}^\dagger, (\hat{a}_{1,2})$  creates (destroys) a particle in modes 1,2, respectively, (modes 1 and 2 referring to the two effective “sides” of the junction). Here,  $N = \hat{n}_1 + \hat{n}_2 = \hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2$  commutes with  $\hat{H}$ , and so may be taken as a  $c$  number. For  $N$  up to the order of  $10^3$  or so it is easy to diagonalize  $\hat{H}$  numerically. This direct approach will afford a check on our results in one limit, but it fails for larger  $N$ , which may be required for experimental observation, but that may nevertheless be within the mesoscopic range. And, of course, a numerical solution affords no conceptual picture that may be applied beyond the idealized model itself.

Before constructing our EQPM, we briefly describe the two alternative theories for this system, which do offer generalizable concepts, and to which our formulation will be compared. In the two-mode version of the Gross-Pitaevskii MFT, we assume that for large enough  $N$ , we can replace the operators  $\hat{a}_j \rightarrow \sqrt{n_j} e^{i\phi_j}$  with  $c$  numbers. Defining the relative phase  $\phi = \phi_1 - \phi_2$  and number  $n = 1/2(n_1 - n_2)$ , we obtain the classical Hamiltonian of a nonrigid pendulum [7]

$$H_{cl} = \frac{E_c}{2} n^2 - E_J \sqrt{1 - \left(\frac{2n}{N}\right)^2} \cos \phi. \quad (2)$$

In this classical theory, there is no difficulty whatever about the fact that  $\phi$  and  $n$  are canonically conjugate, and the canonical equations of motion derived from  $H_{cl}$  are integrable in terms of Jacobi elliptic functions [7]. It will suffice for our purposes to note the motion in the vicinity of the fixed points. The global minimum of  $H_{cl}$  is always  $n = \phi = 0$ ; and orbits about it have frequency  $N^{-1} \sqrt{E_J(4E_J + N^2 E_c)}$ , spanning the range from Bloch to Josephson oscillations as  $N^2 E_c / E_J$  increases. (Note that in dilute Bose-Einstein condensates,  $E_c N$  will be on the order of the chemical potential  $\mu$ , and one can have  $E_J = N\omega/2$  for Bloch frequency  $\omega$  es-

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sentially arbitrary in comparison with  $\mu$ , so that  $N^2 E_c/E_J$  can range from much less to much more than one.) For  $N^2 E_c/E_J < 4$ ,  $(n, \phi) = (0, \pi)$  is a maximum; but for  $N^2 E_c/E_J > 4$  it is a saddle point, and there are two maxima at  $(n, \phi) = (\pm n_m, \pi)$ . The frequency of oscillations about  $(0, \pi)$  (or rate of dynamical instability when it is a saddle-point) is  $N^{-1} \sqrt{E_J(4E_J - N^2 E_c)}$ . And when the two degenerate maxima exist, there are orbits about each of them such that  $n$  is always either positive or negative, and  $\phi$  remains close to  $\pi$  (except possibly for large radius orbits).

If we attempt to go beyond the classical approximation of this MFT, the classical conjugacy of  $\phi$  and  $n$  motivates the standard QPM [12,16–19,21], in which we quantize naively by setting  $(\hat{n}_1 - \hat{n}_2)/2 \rightarrow i(\partial/\partial\phi)$ . This leads to a Schrödinger equation  $i\hbar\Psi = \hat{H}_\phi\Psi$  for the  $2\pi$ -periodic wave-function  $\Psi(\phi)$ , with

$$\hat{H}_\phi = -\frac{E_c}{2} \frac{\partial^2}{\partial\phi^2} - E_J \cos\phi, \quad (3)$$

so that the  $\Psi$  of energy eigenstates are Mathieu functions. Standard inner products  $\langle\Psi|\Psi'\rangle = \oint d\phi \Psi(\phi)^* \Psi'(\phi)$  and expectation values  $\langle\hat{A}\rangle = \oint d\phi \Psi(\phi)^* A(\phi, t) \Psi(\phi)$  are assumed. The problem with this approach is that the naive quantization has in fact been too naive: there are serious problems with making  $\phi$  and  $n$  into canonically commuting operators [20]. And even to obtain (2) from (3) by our naive quantization, we have neglected  $n^2$  in comparison with  $N^2/4$  under the root. This naive approach does allow us, however, to obtain a second-order equation for  $\Psi$ , which is simple enough to be solved exactly as a quantum problem, but that nevertheless reproduces some of the behaviors predicted by the MFT. There can be low-energy Josephson states localized in the well about  $\phi=0$ , and also high-energy running states  $\Psi \sim \exp(\pm ik\phi)$ , corresponding to the MFT orbits (of large radius) about one of the two maxima, having either positive or negative  $n$ . Although the QPM and MFT are both based on large  $N$ , however, some of their predictions differ. If  $E_c/E_J \geq 1$ , the QPM implies that there will be no localized eigenstates, and hence, no small-amplitude Josephson phase oscillations. And although in running states  $|\Psi|^2$  will be slightly larger near  $\phi=\pi$ , the QPM does not allow true  $\pi$  oscillations.

The questions therefore arise, which if either of these theories is correct where they disagree, and what corrections may appear for each in the mesoscopic regime of smaller  $N$ . The convenience and familiarity of the single-particle Schrödinger equation, and the wealth of approximations and generalizations that are available in this context, motivate us to seek a formulation of (1) similar to the QPM; but we will also demand exactness at all  $N$ .

Our construction proceeds as follows. An arbitrary state in the Hilbert space of our two-mode system may be written as

$$|\psi\rangle = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} d\phi_1 d\phi_2 f(\phi_1, \phi_2) |\phi_1, \phi_2\rangle, \quad (4)$$

where the (un-normalized) Bargmann states [22] are

$$|\phi_1, \phi_2\rangle = \sum_{l,m=0}^{\infty} e^{i(l\phi_1 + m\phi_2)} \frac{1}{\sqrt{l!m!}} |l\rangle|m\rangle, \quad (5)$$

with  $|m\rangle, |l\rangle$  being particle number eigenstates of modes 1,2 respectively. (This Bargmann representation is over complete, and from this over completeness arise serious complications in some uses of our EQPM, which may be regarded as the inevitable price of its advantages—a price that will be cheap in some applications, and excessive in others. We will discuss these issues below.) The action of any operators on any state  $|\psi\rangle$  can be represented in terms of differential operators acting on the associated  $f(\phi_1, \phi_2)$ , using

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

$$f(\phi_i) \hat{a}_i^\dagger \rightarrow i \frac{\partial}{\partial\phi_i} [e^{-i\phi_i} f(\phi_i)]. \quad (6)$$

(Simply integrate by parts.) In particular, the number operators assume the familiar forms  $f(\phi_i) \hat{n}_i = f(\phi_i) \hat{a}_i^\dagger \hat{a}_i \rightarrow -i(\partial/\partial\phi_i) f(\phi_i)$ , without any approximation.

For a fixed total number of atoms  $N$ , we may write

$$f(\phi_+ + \phi/2, \phi_+ - \phi/2) = e^{-iN\phi_+} \psi(\phi), \quad (7)$$

with  $\phi_+ = 1/2(\phi_1 + \phi_2)$ , and  $\phi = \phi_1 - \phi_2$  as above. The function  $\psi(\phi)$  is  $2\pi$  (anti-)periodic if  $N$  is (odd) even. Integrating over  $\phi_+$  in Eq. (4) then yields  $|\psi\rangle_N = (1/2\pi) \int_{-\pi}^{\pi} d\phi \psi(\phi) |\phi\rangle$ , for

$$|\phi\rangle = \sum_{n=-N/2}^{N/2} \frac{\exp(in\phi)}{\sqrt{\binom{N}{2+n}! \binom{N}{2-n}!}} |n\rangle$$

$$= N! (\hat{a}_1^\dagger e^{i(\phi/2)} + \hat{a}_2^\dagger e^{-i(\phi/2)})^N |\text{vacuum}\rangle \quad (8)$$

(which may be considered a finite  $N$  generalization of a pure phase state [18]). The action of the Josephson Hamiltonian Eq. (3) on the state vector Eq. (8) may thus be represented as  $\hat{H}|\psi\rangle = (1/2\pi) \int_{-\pi}^{\pi} d\phi |\phi\rangle (\tilde{H}\psi)$  for

$$\tilde{H} \equiv -\frac{E_c}{2} \frac{\partial^2}{\partial\phi^2} - E_J \left(1 + \frac{2}{N}\right) \cos\phi - 2\frac{E_J}{N} \sin\phi \frac{\partial}{\partial\phi}, \quad (9)$$

where (as also in the standard QPM) we have dropped a constant energy shift, in this case  $E_c N(N-2)/8$ . As will be clear after our discussion of over completeness below, the fact that  $\tilde{H}$  is not Hermitian is actually no cause for alarm, because we have maintained Hermiticity within the physical subspace. Because Hermitian Schrödinger equations are more familiar, however, we will finally obtain (1) by defining  $\psi(\phi) = \Psi(\phi) \exp[(2E_J/E_c N) \cos\phi]$ . The result is that we can represent (1) by the EQPM equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[ -\frac{E_c}{2} \frac{\partial^2}{\partial \phi^2} - E_J \left( 1 + \frac{1}{N} \right) \cos \phi - \frac{E_J^2}{N^2 E_c} \cos 2\phi \right] \Psi, \quad (10)$$

dropping another constant  $E_J^2/N^2 E_c$  (just to turn a  $\sin^2 \phi$  term into the  $\cos 2\phi$ ). So, in place of the QPM Mathieu equation, setting  $i\hbar \partial_t \Psi = E \Psi$  in our EQPM gives the three-term Hill equation [23].

Equation (10) is our central result. It is exact, in the sense that the lowest  $N+1$  frequencies in its eigenspectrum are exactly the spectrum of our original two-mode Hamiltonian with fixed  $N$ . (We will show below why only these lowest  $N+1$  states are physical.) Since, in very many cases, it is only this spectrum that is experimentally probed, the subtleties in computing expectation values that are due to the overcompleteness of our representation, will often be irrelevant. Before dealing with those subtleties, therefore, we will first present some deductions from Eq. (10) that are unaffected by them.

We can immediately see that in the limit of large  $N$  for fixed  $E_J/E_c$ , we obtain the standard QPM. Alternatively, in the limit  $E_c \rightarrow 0$ , we recover simple Rabi oscillations, which are described by the MFT but not by the QPM. To see this, we first use time-independent perturbation theory in  $E_c/E_J$  to find the energy of the  $m$ th energy eigenstate of (1) to be

$$\mathcal{E}_m = \mathcal{E}_0 + \left( \frac{E_J}{N} + \frac{NE_c}{4} \right) m - \frac{E_c}{4} m^2 + \mathcal{O}(E_c^2). \quad (11)$$

If we consider Eq. (10) in this same limit  $E_c \rightarrow 0$ , then we can expand the cosines about the two potential minima  $\phi = 0, \pi$ , writing  $\phi = \sqrt{E_c/N} x$  (or  $\phi = \pi - \sqrt{E_c/N} x$ ), to see that to leading order in  $E_c$  we have two harmonic wells, centered on  $\phi = 0, \pi$ , with  $1/E_c$  playing the role of the mass. We may also compute perturbatively the next-to-leading order correction to the energy levels, due to the  $x^4$  anharmonicity. The spectrum for the well at  $\phi = 0$  agrees with Eq. (11), while that for the well at  $\phi = \pi$  is

$$\begin{aligned} \mathcal{E}_m^\pi = \mathcal{E}_0 + (N+1)ft \left( \frac{E_J}{N} - \frac{E_c}{4} \right) + \left( \frac{E_J}{N} - \frac{(N+2)E_c}{4} \right) m \\ - \frac{E_c}{4} m^2 + \mathcal{O}(E_c^2). \end{aligned} \quad (12)$$

Hence, we have  $\mathcal{E}_0^\pi > \mathcal{E}_N$  to  $\mathcal{O}(E_c^2)$ , so that all of the  $N+1$  physical states are in the  $\phi = 0$  well.

If  $E_c/E_J$  is of order  $N^{-2}$ , then we are beyond the Rabi regime, but EQPM still provides corrections to the QPM. Expanding the potential around the two extrema  $\phi = 0, \pi$ , we find the oscillator frequencies  $N^{-1} \sqrt{E_J(4E_J \pm N^2 E_c)}$ , in agreement with the MFT as discussed above, and in contrast to the results  $\sqrt{\pm E_J E_c}$  of the standard QPM. However, one may show that as long as there is a second local minimum at  $\phi = \pi$ , the highest physical state has energy below that minimum. It is therefore not obvious, at this point, how the EQPM admits  $\pi$  states any more than does the QPM. To see

that indeed it does admit them, we must finally address the consequences of Bargmann overcompleteness.

The main consequence of overcompleteness is that the inner product on the EQPM wave function  $\psi(\phi)$  is not the standard one of single-particle quantum mechanics, but the nonlocal

$$\langle \psi | \psi' \rangle = \frac{1}{(2\pi)^2} \oint d\theta \oint d\phi \psi^*(\theta) \psi'(\phi) \langle \theta | \phi \rangle,$$

where

$$\begin{aligned} \langle \theta | \phi \rangle &= \sum_{n=-N/2}^{N/2} \frac{e^{in(\phi-\theta)}}{\left( \frac{N}{2} + n \right)! \left( \frac{N}{2} - n \right)!} = \frac{2^N}{N!} \cos^N \left( \frac{\phi-\theta}{2} \right) \\ &= 2\pi \frac{2^N}{(N!!)^2} \delta_N(\phi-\theta). \end{aligned} \quad (13)$$

In the infinite  $N$  limit,  $\langle \theta | \phi \rangle$  becomes proportional (in the interval  $\phi, \theta \in [-\pi, \pi]$ ) to a delta function

$$\lim_{N \rightarrow \infty} \delta_N(\phi-\theta) = \delta(\phi-\theta), \quad (14)$$

and so for large  $N$ , the nonstandard inner product can often be ignored. Even for very large  $N$ , however, the inner product (13) has the effect of eliminating all Fourier components  $e^{ik\phi}$  having  $|k| > N/2$ . In fact, it is clear from the early step (8) in our derivation that this is as it should be. For higher energies, of order  $N^2 E_c$ , projecting out these unphysical Fourier components can drastically alter the shape of the eigenfunctions. In fact, one may prove, by examining (9) in Fourier space, that projecting out unphysical Fourier components will annihilate all energy eigenfunctions above the lowest  $N+1$ . For the higher physical states, we can use the WKB approximation to (9), to see that the phase of  $\psi(\phi)$  will vary more rapidly near  $\phi = 0$  than near  $\phi = \pi$ , so that the nonvanishing amplitude around  $\phi = 0$  will actually be unphysical, and the physical part of  $\psi(\phi)$  will be concentrated around  $\phi = \pi$ .

This effect can be shown quantitatively by computing  $\langle \alpha, \phi_0, N | \Psi \rangle$ , where  $\sqrt{N!} |\alpha, \phi_0, N\rangle = (\hat{a}_1^\dagger e^{i\phi_0/2} \cos(\alpha/2) + \hat{a}_2^\dagger e^{-i\phi_0/2} \sin(\alpha/2))^N |\text{vac}\rangle$  is the SU(2) coherent state on which the number-conserving MFT is based. In the energy range where the MFT predicts  $\pi$  states, we can use WKB for  $\psi(\phi)$ , and for large  $N$ , we can evaluate the inner product using steepest descents. The result confirms the MFT prediction. An exception is the extreme high- $N$  limit  $N^2 E_c > 2NE_J$ , where we may see from the WKB approximation to  $\psi(\phi)$  that its wave number does not vary significantly with  $\phi$ , and so projecting out unphysical frequencies either annihilates eigenfunctions entirely, or else has little effect on them. Consequently, there are no  $\pi$  states in this regime, and the standard QPM is essentially vindicated over MFT, even at very high  $N$ : the usual  $N^{-1/2}$  improvement in MFT accuracy is overwhelmed by strong number squeezing due to the predominance of the nonlinear interaction [24].

In conclusion, we have derived an exact version of the phenomenological quantum phase model, from the two-mode Bose-Hubbard model for a Josephson junction. We have shown that this exact quantum phase model reproduces the time scales and (except for very large  $N$ ) the  $\pi$  states of the Gross-Pitaevskii mean-field theory. The corrections we find to the standard QPM include a  $\cos 2\phi$  term in the potential, and the fact that the inner product must be nonlocal in  $\phi$ , because of the need to project out unphysically high Fourier components in the wave functions. For some compu-

tations, the nonlocal inner product may introduce too severe complications; but in general, our formalism, and its generalizations, should provide valuable additional tools for understanding quantum effects in mesoscopic Josephson systems.

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