

# Semiclassical quantization for a bosonic atom-molecule conversion system

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(Received 13 May 2015; published 27 July 2015)

We consider a simple quantum model of atom-molecule conversion where bosonic atoms can combine into diatomic molecules and vice versa. The many-particle system can be expressed in terms of the generators of a deformed  $su(2)$  algebra, and the mean-field dynamics takes place on a deformed version of the Bloch sphere, a teardrop shaped surface with a cusp singularity. We analyze the mean-field and many-particle correspondence, which shows typical features of quantum-classical correspondence. We demonstrate that semiclassical methods can be employed to recover full many-particle features from the mean-field description in cold atom systems with atom-molecule conversion, and we derive an analytic expression for the many-particle density of states in the limit of large particle numbers.

DOI: [10.1103/PhysRevA.92.012121](https://doi.org/10.1103/PhysRevA.92.012121)

PACS number(s): 03.65.Sq, 03.75.-b, 05.30.Jp

## I. INTRODUCTION

The experimental progress in confining and manipulating cold atoms and Bose-Einstein condensates (BECs) offers a unique opportunity to investigate the quantum properties of interacting many-particle systems. For most realistic setups, however, a theoretical full many-particle description is beyond the current state of the art. Most commonly the mean-field approximation is applied, resulting in a description of the many-particle system by an effective single-particle wave function. The time evolution is in this description governed by a nonlinear Schrödinger equation. This approximation is closely related to the classical limit of single-particle quantum systems, where the particle number plays the role of  $\hbar^{-1}$ . Recently there have been several studies demonstrating that this analogy can be used to apply semiclassical techniques to recover full many-particle features from the mean-field description alone [1–6].

Over the last decade there has been considerable interest in atom-molecule conversion in cold atoms and BECs [7–17]. Theoretically these systems are closely related to deformed  $su(m)$  algebras [18]. Neglecting quantum fluctuations in the many-particle dynamics leads to mean-field approximations defined on phase spaces with nonstandard geometries, and new interesting features in the many-particle and mean-field correspondence. Here we address the question of whether semiclassical methods might be adapted to describe the full many-particle behavior of atom-molecule conversion systems on the grounds of their mean-field approximation.

We focus on the simplest model of an atom-molecule conversion system, similar to the one considered in [7], consisting of noninteracting atoms and diatomic molecules each of which can populate only one mode. Introducing the atomic and molecular creation and annihilation operators  $\hat{a}^\dagger$ ,  $\hat{a}$  and  $\hat{b}^\dagger$ ,  $\hat{b}$ , respectively, this system can be described by a Hamiltonian of the form

$$\hat{H} = \epsilon_a \hat{a}^\dagger \hat{a} + \epsilon_b \hat{b}^\dagger \hat{b} + \frac{v}{2\sqrt{N}} (\hat{a}^\dagger \hat{a}^\dagger \hat{b} + \hat{a} \hat{a} \hat{b}^\dagger), \quad (1)$$

where  $\epsilon_{a,b}$  is the energy of the atomic or molecular mode, and  $v$  describes the conversion strength between atoms and molecules. The total number of atoms  $\hat{N} = \hat{a}^\dagger \hat{a} + 2\hat{b}^\dagger \hat{b}$  is a constant of motion. For a fixed value of the particle number  $N$

the system lives on an  $[\frac{N}{2}]_+ + 1$ -dimensional Hilbert space. For simplicity, we confine the discussions to even particle numbers in what follows.

We begin with a review of the many-particle and mean-field descriptions, and their correspondence. Then we introduce a semiclassical quantization condition and demonstrate that the many-particle spectrum can be accurately recovered from the mean-field dynamics, and derive an analytic expression for the many-particle density of states in the semiclassical limit of large particle numbers. We also present results for the semiclassical many-particle eigenstates. We end with a summary and outlook.

## II. THE MANY-PARTICLE SYSTEM

Similar to the two-mode Bose-Hubbard model [19], we can apply a Schwinger-type transformation to introduce the operators

$$\begin{aligned} \hat{K}_x &= \frac{\hat{a}^\dagger \hat{a}^\dagger \hat{b} + \hat{a} \hat{a} \hat{b}^\dagger}{2\sqrt{N}}, \\ \hat{K}_y &= \frac{\hat{a}^\dagger \hat{a}^\dagger \hat{b} - \hat{a} \hat{a} \hat{b}^\dagger}{2i\sqrt{N}}, \\ \hat{K}_z &= \frac{\hat{a}^\dagger \hat{a} - 2\hat{b}^\dagger \hat{b}}{4}. \end{aligned} \quad (2)$$

The Hamiltonian can then be expressed as

$$\hat{H} = \epsilon \hat{K}_z + v \hat{K}_x, \quad (3)$$

where we have shifted the zero energy and introduced the parameter  $\epsilon = 2\epsilon_a - \epsilon_b$ .

The physical meaning of the operators  $\hat{K}_j$  is similar to the two-mode Bose-Hubbard case. That is,  $\hat{K}_z$  measures the population imbalance between molecular and atomic mode, and  $\hat{K}_{x,y}$  measure their phase relation. It is further convenient to introduce the operators

$$\hat{K}_\pm = \hat{K}_x \pm i\hat{K}_y, \quad (4)$$

that create a molecule out of two atoms and vice versa. The operators (2) and (4) are related to a *nonlinear deformation* of an  $su(2)$  algebra [18,20,21]. That is, they fulfill commutation

relations of the form

$$[\hat{K}_z, \hat{K}_\pm] = \pm \hat{K}_\pm, \quad (5)$$

just as for  $\text{su}(2)$ , and

$$[\hat{K}_+, \hat{K}_-] = F(\hat{K}_z, \hat{N}), \quad (6)$$

where  $F(\hat{K}_z, \hat{N})$  is a polynomial in  $\hat{K}_z$  and  $\hat{N}$ . Specifically we have

$$F(\hat{K}_z, \hat{N}) = -\frac{\hat{N}}{N} - \frac{1}{4N}(\hat{N} + 4\hat{K}_z)(\hat{N} - 12\hat{K}_z). \quad (7)$$

In terms of  $\hat{K}_x$ ,  $\hat{K}_y$ , and  $\hat{K}_z$  the commutation relations read

$$[\hat{K}_z, \hat{K}_x] = i\hat{K}_y, \quad (8)$$

$$[\hat{K}_y, \hat{K}_z] = i\hat{K}_x, \quad (9)$$

$$[\hat{K}_x, \hat{K}_y] = \frac{i}{2}F(\hat{K}_z, \hat{N}). \quad (10)$$

The total particle number  $\hat{N}$  commutes with  $\hat{K}_x$ ,  $\hat{K}_y$ , and  $\hat{K}_z$ . In the case of a Bose-Hubbard dimer the conserved particle number reflects the conservation of the total angular momentum. For deformed  $\text{su}(2)$  algebras this is replaced by a less trivial conservation law. We can find the conserved quantity using the approach in [18] as

$$\begin{aligned} \hat{C} &= \hat{K}_- \hat{K}_+ + \frac{4}{N} \hat{K}_z^3 + \frac{\hat{N} + 6}{N} \hat{K}_z^2 + \frac{8 - \hat{N}^2}{4N} \hat{K}_z \\ &= \hat{K}_x^2 + \hat{K}_y^2 + \frac{4}{N} \hat{K}_z^3 + \frac{\hat{N}}{N} \hat{K}_z^2 \\ &\quad + \frac{8 - \hat{N}^2 - 4\hat{N}}{4N} \hat{K}_z + \frac{4\hat{N} + \hat{N}^2}{8N}. \end{aligned} \quad (11)$$

Evaluating  $\langle \hat{C} \rangle$  in any eigenstate of  $\hat{K}_z$  yields the conservation law

$$\begin{aligned} \langle \hat{K}_x^2 \rangle + \langle \hat{K}_y^2 \rangle &= -\frac{2\langle \hat{K}_z \rangle}{N} + \frac{\langle \hat{N} \hat{K}_z \rangle}{N} + \frac{\langle \hat{N}^2 \hat{K}_z \rangle}{4N} \\ &\quad - \frac{\langle \hat{N} \hat{K}_z^2 \rangle}{N} - \frac{4\langle \hat{K}_z^3 \rangle}{N} + \frac{N^2}{16} + \frac{N}{4}. \end{aligned} \quad (12)$$

We shall see later that this corresponds to a deformation of the familiar Bloch sphere of two-level systems to a teardrop shape on which the mean-field dynamics take place.

From the commutation relation (5) it follows that  $\hat{K}_+$  and  $\hat{K}_-$  are the usual lowering and raising operators for  $\hat{K}_z$ , from which one can deduce that the spectrum of  $\hat{K}_z$  is equidistant [18]. For a given even particle number  $N$  the eigenvalues of  $\hat{K}_z$  run in integer steps from  $-\frac{N}{4}$  to  $\frac{N}{4}$ .

While due to symmetry the operators  $\hat{K}_x$  and  $\hat{K}_y$  are isospectral, their spectrum differs from that of  $\hat{K}_z$  and, in particular, is not equidistant. The spectrum is depicted for the example  $N = 50$  in Fig. 1. It can be seen that the eigenvalues are symmetric around zero, and approximately equidistant at the boundaries of the spectrum, while they are closer together around the center. The eigenvalues can be obtained analytically using a Bethe ansatz approach [12].

Figure 2 depicts the eigenvalues of the many-particle Hamiltonian (3) as a function of  $\epsilon$  for  $v = 1$ , and two different

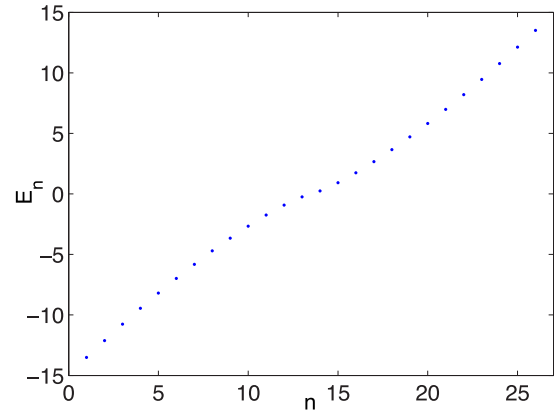


FIG. 1. (Color online) Eigenvalues of  $\hat{K}_x$  (and  $\hat{K}_y$ ) for  $N = 50$ .

particle numbers. In comparison to the familiar Landau-Zener behavior of a many-particle two-level system without atom-molecule conversion, the simple symmetry with respect to  $\epsilon$  is lost, and we observe a cluster of narrow avoided crossings for intermediate values of  $\epsilon$ , stretching from the upper end of the spectrum for negative values of  $\epsilon$  to the lower one for positive values. These are the reflection of the accumulation of eigenvalues in the spectrum of  $\hat{K}_x$  in Fig. 1. For large values of  $\epsilon$  the many-particle spectrum is dominated by the equidistant spectrum of  $\hat{K}_z$ . The narrow avoided crossings lead to quasistationary states related to unstable stationary states in

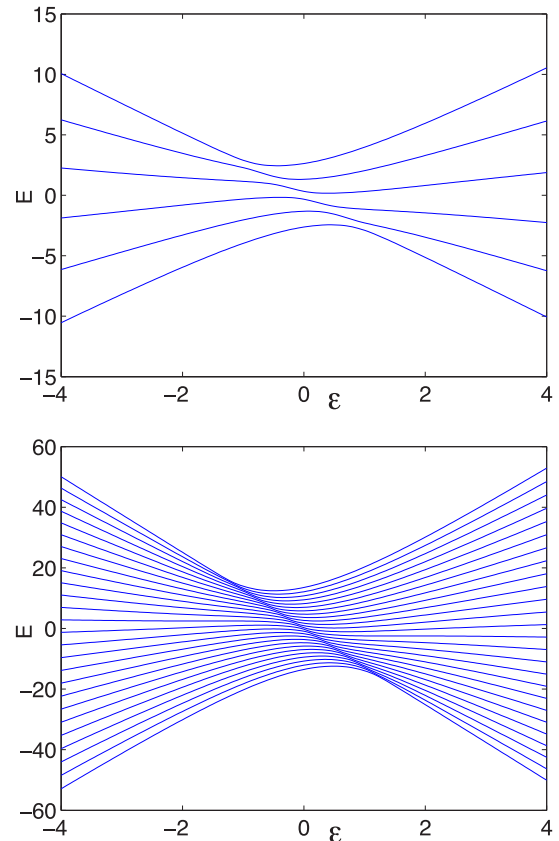


FIG. 2. (Color online) Many-particle spectrum in dependence on  $\epsilon$  for  $v = 1$  and  $N = 10$  (top) and  $N = 50$  (bottom) particles.

the mean-field description. These are related to the molecular mode, where all particles are paired up in diatomic molecules.

The many-particle dynamics can be straightforwardly obtained by integration of the Schrödinger equation on the  $(\frac{N}{2} + 1)$ -dimensional Hilbert space. It is nevertheless instructive to study the Heisenberg equations of motion for the dynamical variables  $\hat{K}_{x,y,z}$ , given by

$$\begin{aligned} \frac{d}{dt} \hat{K}_x &= -\epsilon \hat{K}_y, \\ \frac{d}{dt} \hat{K}_y &= \epsilon \hat{K}_x + \frac{v}{2} + \frac{v}{8N} (\hat{N}^2 - 8\hat{K}_z \hat{N} - 48\hat{K}_z^2), \\ \frac{d}{dt} \hat{K}_z &= v \hat{K}_y. \end{aligned} \quad (13)$$

Due to the nonlinearity of the commutator of  $\hat{K}_x$  and  $\hat{K}_y$  this is not a closed set of equations if  $v \neq 0$ , that is, the right-hand side contains dynamical variables such as  $\hat{K}_z^2$  whose dynamics is not determined by the dynamical equations (13). In the trivial case  $v = 0$ , where the atomic and molecular mode decouple, we have a closed set of equations, describing rigid rotations around the  $z$  axis. In the general case, taking the expectation value and neglecting quantum fluctuations, i.e., approximating expectation values of products with products of expectation values, yields the mean-field approximation we shall discuss in the following section. It is interesting to note that the same dynamical equations in terms of generators of a deformed  $su(2)$  algebra also appear in the context of fermionic atom-molecule conversion [10,22].

### III. MEAN-FIELD APPROXIMATION

In this section we review the derivation of the mean-field dynamics, and summarize its most important features [8–17]. Here we formulate the approximation in a way that is most natural from the perspective of a semiclassical limit. The mean-field approximation can be obtained in the limit of large Hilbert-space dimension by replacing expectation values of products with products of expectation values in the dynamics of the operators  $\hat{K}_j$  in Eq. (13). Introducing the mean-field variables  $s_j = \eta \langle \hat{K}_j \rangle$ , with  $\eta = (\frac{N}{2} + 1)^{-1} \rightarrow 0$ , the mean-field dynamical equations become

$$\begin{aligned} \dot{s}_x &= -\epsilon s_y, \\ \dot{s}_y &= \epsilon s_x + \frac{v}{4} (1 - 4s_z - 12s_z^2), \\ \dot{s}_z &= v s_y. \end{aligned} \quad (14)$$

These can be formulated as canonical Hamiltonian dynamics with the classical Hamiltonian function

$$H = \eta \langle \hat{H} \rangle = \epsilon s_z + v s_x, \quad (15)$$

and the Poisson brackets

$$\begin{aligned} \{s_x, s_y\} &= \frac{1}{4} (1 - 4s_z - 12s_z^2), \\ \{s_y, s_z\} &= -s_x, \\ \{s_z, s_x\} &= -s_y, \end{aligned} \quad (16)$$

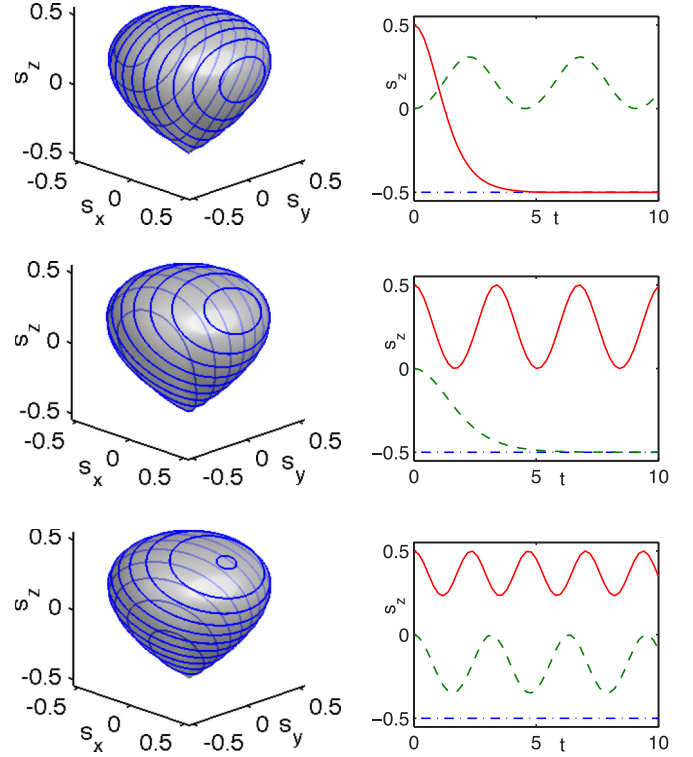


FIG. 3. (Color online) Mean-field dynamics on the deformed Bloch sphere for  $v = 1$  and  $\epsilon = 0, 1, 2$  (from top to bottom). The right panel shows the dynamics of  $s_z$  for selected initial conditions.

which directly follow from the many-particle commutators with the identification

$$\{s_j, s_k\} = \lim_{N \rightarrow \infty} i \eta \langle [\hat{K}_j, \hat{K}_k] \rangle. \quad (17)$$

The dynamics (14) is confined to a two-dimensional surface given by the constraint

$$s_x^2 + s_y^2 = \frac{1}{4} (1 - 2s_z)(1 + 2s_z)^2 =: r^2(s_z), \quad (18)$$

with  $s_z \in [-\frac{1}{2}, \frac{1}{2}]$ . This constraint also follows from the many-particle conserved quantity (12) in the mean-field limit. The resulting surface is depicted in Fig. 3. It has a characteristic inverted teardrop shape, with a tip at  $s_z = -\frac{1}{2}$ . Note that similar shapes are known as Kummer shapes in the classical description of coupled oscillators of different frequencies [23–25].

From the dynamical equations (14) it follows that all fixed points are located at  $s_y = 0$ , and have to fulfill

$$\epsilon s_x = -\frac{v}{4} \left( \frac{1}{2} + s_z \right) (2 - 12s_z). \quad (19)$$

Using the constraint (18) this yields a polynomial in the  $s_z$  component of the fixed points

$$\left( \frac{1}{2} + s_z \right)^2 \left[ \frac{v^2}{4} - \epsilon^2 - (3v^2 - 2\epsilon^2)s_z + 9v^2 s_z^2 \right] = 0. \quad (20)$$

It can be verified that for each of the solutions  $s_z \in [-\frac{1}{2}, \frac{1}{2}]$  of Eq. (20) there is one corresponding value for  $s_x$  such that the dynamics is stationary. That is, there is always a fixed point at the tip of the teardrop, at  $s_z = -\frac{1}{2}$ . Depending on the values of

$v$  and  $\epsilon$  there can be one or two further fixed points. For values of  $\epsilon$  that are smaller than a critical value  $|\epsilon_{\text{crit}}| = \sqrt{2}|v|$  there are three fixed points. A stability analysis reveals that the fixed point at the tip of the teardrop is a saddle point in this case, while the other two fixed points are elliptic. At the critical value  $|\epsilon_{\text{crit}}| = \sqrt{2}|v|$  one of the other two fixed points collides with the fixed point at the tip of the teardrop and then moves to unphysical values  $s_z < -\frac{1}{2}$ . The two fixed points interchange their stability in this transcritical bifurcation. That is, for values of  $\epsilon$  larger than the critical value there are two elliptic fixed points, one of which is located at the tip, the other elsewhere on the teardrop. Examples of the dynamics for  $v = 1$  and different values of  $\epsilon$  are shown in Fig. 3. In the top two figures the fixed point at the tip of the teardrop is a saddle point, which is approached asymptotically by trajectories starting in a particular region on the teardrop, that shrinks as  $\epsilon$  gets closer to the critical value. In the lowest figure the value of  $\epsilon$  is supercritical, and we observe the typical oscillations for trajectories in the neighborhood of the elliptic fixed point at the tip of the teardrop.

We can introduce a set of canonical variables  $p$  and  $q$  via the transformation

$$s_x = r(p) \cos(q), \quad (21)$$

$$s_y = r(p) \sin(q), \quad (22)$$

$$s_z = p, \quad (23)$$

with  $r(p) = \frac{\sqrt{(1-2p)(1+2p)^2}}{2}$ , with  $p \in [-\frac{1}{2}, \frac{1}{2}]$  and  $q \in [0, 2\pi]$ . It is straightforward to verify that this indeed recovers the Poisson brackets (16) with the standard definition

$$\{A, B\} := \frac{\partial A}{\partial p} \frac{\partial B}{\partial q} - \frac{\partial A}{\partial q} \frac{\partial B}{\partial p}. \quad (24)$$

In terms of  $p$  and  $q$  the dynamics is then given by the canonical equations  $\dot{q} = \frac{\partial H}{\partial p}$  and  $\dot{p} = -\frac{\partial H}{\partial q}$  with the Hamiltonian function (15) expressed in terms of  $p$  and  $q$ :

$$H = \epsilon p + \frac{v}{2} \sqrt{(1-2p)(1+2p)^2} \cos(q). \quad (25)$$

The mean-field dynamics can of course be expressed in terms of a nonlinear Schrödinger equation for an effective single-particle wave function. In the case of atom-molecule conversion there are two natural ways to define a mean-field wave function. The first, most commonly used, arises via the usual identification of the components of the mean-field wave function with the probability amplitudes to be in one of the states, in this case to be in the atomic or molecular state. That is, we make the identification  $\hat{a}^{(\dagger)} \rightarrow \frac{1}{\sqrt{\eta}} \psi_a^{(*)}$ , and  $\hat{b}^{(\dagger)} \rightarrow \frac{1}{\sqrt{\eta}} \psi_b^{(*)}$ . The resulting mean-field wave function is then normalized as  $|\psi_a|^2 + 2|\psi_b|^2 = 2$ , where  $|\psi_a|^2/2$  is the probability to find the mean-field system in the atomic mode and  $|\psi_b|^2$  is the probability to find it in the molecular mode. The mean-field dynamics is then governed by the Hamiltonian dynamics

$$i\hbar\dot{\psi}_j = \frac{\partial H}{\partial \psi_j^*}, \quad (26)$$

with the Hamiltonian function  $H$  expressed in terms of the  $\psi_j$  as

$$H = \frac{\epsilon}{4} (|\psi_a|^2 - 2|\psi_b|^2) + \frac{v}{2\sqrt{2}} (\psi_a^{*2} \psi_b + \psi_a^2 \psi_b^*), \quad (27)$$

that is,

$$i \begin{pmatrix} \dot{\psi}_a \\ \dot{\psi}_b \end{pmatrix} = \begin{pmatrix} \frac{\epsilon}{4} & \frac{v}{\sqrt{2}} \psi_a^* \\ \frac{v}{2\sqrt{2}} \psi_a & -\frac{\epsilon}{2} \end{pmatrix} \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix}. \quad (28)$$

With the identification

$$\begin{aligned} s_x &= \frac{1}{2\sqrt{2}} (\psi_a^{*2} \psi_b + \psi_b^* \psi_a^2), \\ s_y &= \frac{1}{2\sqrt{2}i} (\psi_a^{*2} \psi_b - \psi_b^* \psi_a^2), \\ s_z &= \frac{1}{4} (|\psi_a|^2 - 2|\psi_b|^2), \end{aligned} \quad (29)$$

this yields the dynamical equations (14) as expected.

Alternatively, we can replace  $\hat{a}^{2(\dagger)} \rightarrow \frac{1}{\eta} \chi_a^{(*)}$ , and  $\hat{b}^{(\dagger)} \rightarrow \frac{1}{\sqrt{\eta}} \chi_b^{(*)}$ . Then we have  $|\chi_a| + 2|\chi_b|^2 = 2$ , and the nonlinear Schrödinger equation follows from the many-particle dynamics as

$$i \begin{pmatrix} \dot{\chi}_a \\ \dot{\chi}_b \end{pmatrix} = \begin{pmatrix} \frac{\epsilon}{2} & \sqrt{2}v|\chi_a| \\ \frac{v}{2\sqrt{2}} & -\frac{\epsilon}{2} \end{pmatrix} \begin{pmatrix} \chi_a \\ \chi_b \end{pmatrix}. \quad (30)$$

In this version the probability to find the system in the atomic mode is given by  $|\chi_a|/2$ , while the probability to find the system in the molecular mode is  $|\chi_b|^2$ . The variables  $s_j$  are then defined as

$$\begin{aligned} s_x &= \frac{1}{2\sqrt{2}} (\chi_a^* \chi_b + \chi_b^* \chi_a), \\ s_y &= \frac{1}{2\sqrt{2}i} (\chi_a^* \chi_b - \chi_b^* \chi_a), \\ s_z &= \frac{1}{4} (|\chi_a| - 2|\chi_b|^2). \end{aligned} \quad (31)$$

Their dynamics are again given by Eq. (14).

#### IV. MEAN-FIELD AND MANY-PARTICLE CORRESPONDENCE

Let us first compare the spectral features of the mean-field and many-particle descriptions. For this purpose we define the mean-field energies as the values of the Hamiltonian function in the mean-field fixed points, that correspond to stationary solutions of the nonlinear Schrödinger equation. The resulting mean-field energies are plotted as a function of  $\epsilon$  for  $v = 1$  in comparison with the many-particle energies for  $N = 30$  particles in Fig. 4. It can be clearly seen how the pattern of narrow avoided crossings in the many-particle spectrum is closely following one of the mean-field energies. This energy corresponds to the unstable fixed point at the tip of the teardrop that is associated to the all-molecular mode. At the critical values of  $\epsilon = \pm\sqrt{2}$  this becomes a stable elliptic fixed point, that is associated to the minimum and maximum eigenvalues of the many-particle system, respectively. The maximum and minimum mean-field energies bound the many-particle spectrum, if the latter is renormalized by the semiclassical



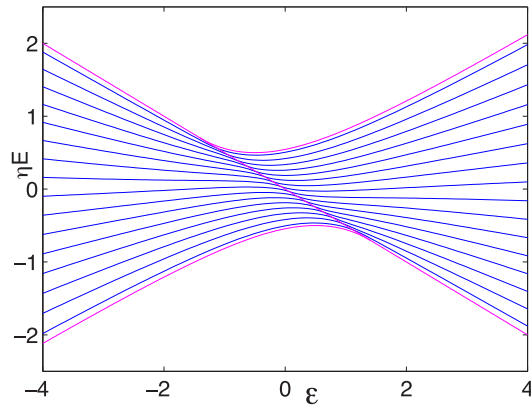


FIG. 4. (Color online) Many-particle [blue (dark gray)] and mean-field [magenta (light gray)] energies in dependence on  $\epsilon$  for  $v = 1$  and  $N = 30$  particles.

parameter  $\eta$ , as is expected in a typical quantum-classical correspondence. This is very promising for a semiclassical quantization that we shall attempt in the next section.

Let us now briefly turn to the correspondence between mean-field and many-particle dynamics. In Fig. 5 we show several examples of mean-field trajectories (black lines) for different parameter values and initial conditions, in comparison to the corresponding many-particle dynamics. For comparison the initial many-particle state has been chosen as the ground state of a Hamiltonian of the type

$$\hat{K} = a\hat{K}_x + b\hat{K}_z + c\hat{K}_y, \quad (32)$$

whose expectation values of  $\hat{K}_{x,y,z}$  lie as close as possible to the teardrop surface of the mean-field system. In Fig. 6 we show the expectation values of  $\hat{K}_x$  and  $\hat{K}_z$  for this family of states for  $c = 0$  and varying values of  $a$  and  $b$ , for different

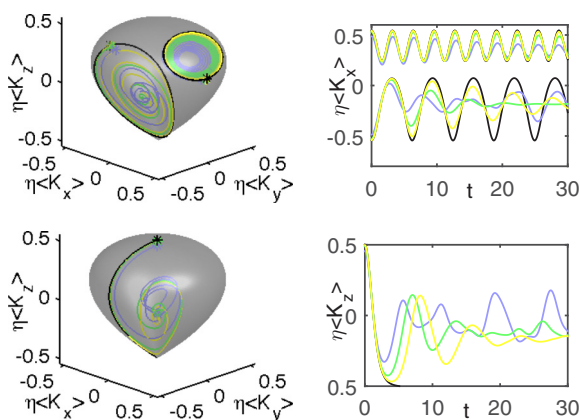


FIG. 5. (Color online) Mean-field (black) and many-particle dynamics for  $v = 1$  and  $\epsilon = 1$  (top) and  $\epsilon = 0$  (bottom), and different particle numbers. The blue (dark gray), green (gray), and yellow (light gray) curves correspond to  $N = 20, 100,$  and  $500$ , respectively. The initial states are chosen as the ground states of  $\pm\hat{K}_x$  in the top figure and  $-\hat{K}_z$  in the bottom figure, and the initial conditions are marked by a star. The right figure on the top shows the dynamics of the  $x$  component for  $\epsilon = 1$ , and the figure on the bottom right shows the dynamics of the  $z$  component for  $\epsilon = 0$ .

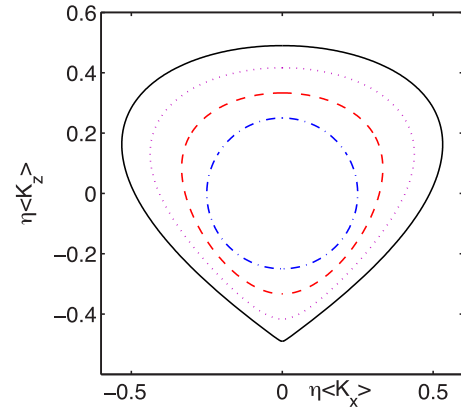


FIG. 6. (Color online) Expectation values of  $\hat{K}_x$  and  $\hat{K}_z$  for the ground states of the Hamiltonian (32) where  $c = 0$ ,  $b$  varies from  $-0.5$  to  $0.5$  and  $a = \pm\frac{1}{2}\sqrt{(1-2b)(1+2b)^2}$ , for different particle numbers  $N = 2$  (blue dash-dotted line),  $N = 4$  (red dashed line),  $N = 10$  (magenta dotted line), and  $N = 100$  (black solid line).

particle numbers. It can be seen how the mean-field teardrop is approached with increasing particle number. See [14] for a comparison between these states and a new type of coherent states proposed there.

In the upper panel of Fig. 5 it can be seen how the many-particle dynamics closely follows the mean-field dynamics even for relatively small particle numbers in the vicinity of elliptic fixed points. Where the influence of the hyperbolic fixed point at the bottom of the teardrop is stronger, the deviations become larger and we observe the typical breakdown phenomenon of the many-particle dynamics. For longer times (not depicted), revival phenomena occur where the revival time rapidly increases with the particle number as expected [19]. The slow convergence of the many-particle dynamics towards the mean-field dynamics is particularly pronounced for those initial states whose mean-field dynamics asymptotically approaches the saddle point related to the all-molecular mode, as seen at the bottom in Fig. 5. The breakdown happens very rapidly here, and even for longer times no revivals are observed. This behavior has been investigated in some detail in [7], and is typical for quantum-classical correspondence in the neighborhood of hyperbolic fixed points.

## V. SEMICLASSICAL QUANTIZATION

In the following we shall investigate how semiclassical techniques might be modified to obtain an approximation for the many-particle eigenvalues from the mean-field dynamics. For this purpose it is convenient to use the approach by Braun [26] that has been developed for general three-term recurrence relations, since the matrix representation of our many-particle Hamiltonian (3) in the eigenbasis of  $\hat{K}_z$  is tridiagonal, and thus the eigenvalue equation defines a three-term recurrence relation. The same procedure has been successfully applied to the spectrum of the two-mode Bose-Hubbard model in [1,2,5]. Since the spectrum of  $\hat{K}_z$  is related to that of two coupled harmonic oscillators, we expect that the semiclassical quantization should yield exact results for the spectrum of  $\hat{K}_z$  for arbitrary particle numbers. For this purpose the

quantization procedure of Braun has to be slightly modified. We shall give a brief overview over this modified version in what follows.

The main idea is to derive a WKB type approximation for the wave function in dependence on  $p$ ; the matching conditions between the allowed and forbidden regions then yield a Bohr-Sommerfeld type quantization condition for the eigenvalues. The latter quantization condition can in fact be motivated heuristically, by arguing that every many-particle state takes up on average a phase-space volume of  $h$ , where the ground state and the highest excited state only take up the minimum uncertainty volume of  $\frac{h}{2}$ . However, the role of the semiclassical parameter  $h$  in the present context is taken over by the inverse matrix size of the problem, that is,  $\eta = (\frac{N}{2} + 1)^{-1}$ . The quantization condition then reads

$$S(\eta E_n) = 2\pi\eta(n + \frac{1}{2}), \quad (33)$$

where  $S(E)$  is the mean-field phase-space area enclosed by the orbit of energy  $E$ . To calculate these phase-space areas it is convenient to introduce potential curves for  $p$ . These potential curves  $U^+$  and  $U^-$  are defined as the maximum and minimum functions of the Hamiltonian with respect to the angle dimension [26]. That is, we have

$$U^\pm(p) = \epsilon p \pm \frac{v}{2}\sqrt{(1-2p)(1+2p)^2}, \quad (34)$$

which join at  $p = \pm\frac{1}{2}$ , at the values  $\pm\frac{\epsilon}{2}$ . Two examples of the potential curves together with the corresponding phase-space portraits are shown in Fig. 7. The potential curves bound the possible values of the energy of the mean-field system for a given value of  $p$ . On the other hand, for a given value of the energy, the motion is restricted to values of  $p$  where  $U^-(p) \leq E \leq U^+(p)$ , i.e., the classically allowed region. This region is bound by the classical turning points  $p_\pm$ , where  $E = U^\pm(p_\pm)$ ,

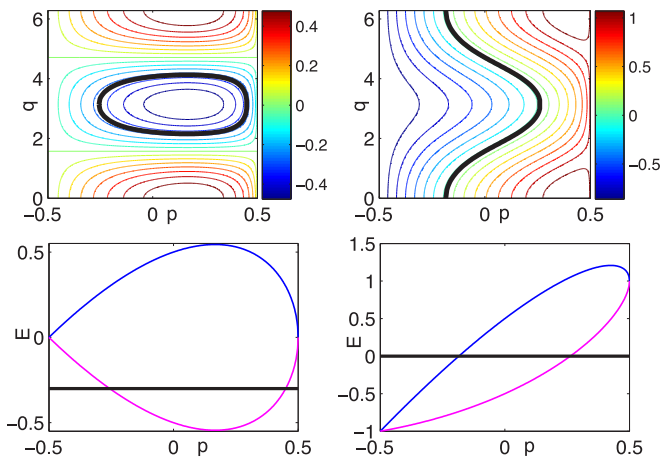


FIG. 7. (Color online) Mean-field phase-space portraits (top) and potential curves (bottom) for  $v = 1$  and  $\epsilon = 0$  (left) and  $\epsilon = 2$  (right). The false colors in the phase-space plots represent the energy values. An orbit belonging to one selected energy each (marked by a black line in the bottom pictures) is highlighted in each of the phase-space plots by a thick black line.

which are found as the two roots of the polynomial

$$2v^2 p^3 + (v^2 + \epsilon^2)p^2 - \left(\frac{v^2}{2} + 2\epsilon E\right)p - \frac{v^2}{4} + E^2, \quad (35)$$

that fall into the interval  $[-\frac{1}{2}, \frac{1}{2}]$ . For any allowed value of the energies the polynomial has three real roots, two of which are located in the interval  $[-\frac{1}{2}, \frac{1}{2}]$ . The third root,  $p_0$ , lies outside the physically relevant interval, to the left, that is,  $p_0 \leq -\frac{1}{2} \leq p_-$ . The fixed points of the dynamics correspond to the extrema of the potential curves and the tip at which both potential curves meet at  $p = -\frac{1}{2}$ . For the extremal values of the energy the two turning points coalesce.

The phase-space area enclosed by an orbit with energy  $E$  can be written as the integral

$$S(E) = \oint q(p, E) dp, \quad (36)$$

where  $q(p)$  follows from the conservation of the energy as

$$q(p) = \arccos\left(\frac{2(E - \epsilon p)}{\sqrt{(1-2p)(1+2p)^2}}\right), \quad (37)$$

and care has to be taken that the area enclosed by the curve is calculated, rather than the area outside the curve. Depending on which turning point lies on which potential curve, the enclosed area in Eq. (36) can be evaluated as

$$S(E) = \begin{cases} 2\pi(p_+ - p_-) - 2\tilde{S}(E), & p_\pm \text{ on } U_- \\ 2\pi(\frac{1}{2} - p_-) - 2\tilde{S}(E), & p_- \text{ on } U_-, p_+ \text{ on } U_+ \\ 2\pi(\frac{1}{2} + p_+) - 2\tilde{S}(E), & p_- \text{ on } U_+, p_+ \text{ on } U_- \\ -2\pi + 2\tilde{S}(E), & p_\pm \text{ on } U_+ \end{cases} \quad (38)$$

with

$$\tilde{S}(E) = \int_{p_-}^{p_+} q(p) dp. \quad (39)$$

In the case  $v = 0$  this can be evaluated analytically, and we obtain the exact eigenvalues for arbitrary particle numbers, as expected. For nonzero values of  $v$  the quantization condition (33) can be straightforwardly solved numerically to obtain the semiclassical many-particle spectrum from the mean-field dynamics. In Fig. 8 we show the resulting semiclassical eigenvalues in dependence on  $\epsilon$  for  $v = 1$  and two different particle numbers, in comparison to the numerically exact many-particle energies. We observe that even for  $N = 4$  particles, corresponding to a relatively large value of  $\eta = \frac{1}{3}$ , the agreement is very good. As expected the quality of the approximation improves with larger particle number. It also improves with larger  $\epsilon$ , as in the limit  $v/\epsilon \rightarrow 0$  the quantization yields exact results.

The quantization condition can be used to derive an analytic expression for the many-particle density of states in the semiclassical limit of large particle numbers [27,28]. Differentiating the quantization condition (33) with respect to the energy yields

$$\frac{dS(E_n)}{dE} = 2\pi \frac{dn}{dE}. \quad (40)$$

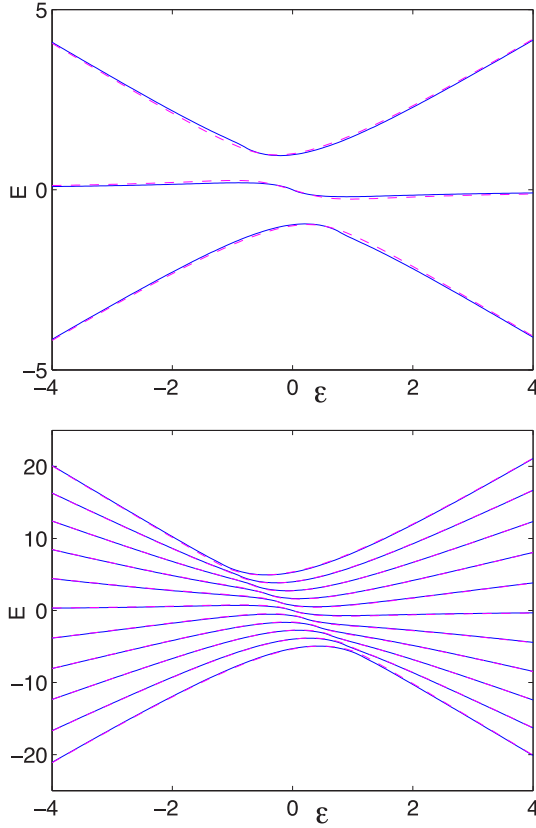


FIG. 8. (Color online) Many-particle (solid blue lines) and semi-classical (dashed magenta lines) eigenvalues in dependence on  $\epsilon$  for  $v = 1$  and two different particle numbers. The upper panel corresponds to  $N = 4$  particles; the lower panel corresponds to  $N = 20$ .

That is, the many-particle density of states is given by the derivative of the mean-field phase-space area with respect to the energy. This, on the other hand, is given by the period of the mean-field orbit of the given energy [29]. That is, we have for the many-particle density of states

$$\frac{dn}{dE} = \frac{T(E)}{2\pi}, \quad (41)$$

where  $T(E)$  denotes the period of the orbit with energy  $E$ . This can be directly calculated from

$$\begin{aligned} T(E) &= 2 \int_{p_-}^{p_+} \frac{dp}{\dot{p}} = 2 \int_{p_-}^{p_+} \left( \frac{\partial H}{\partial q} \right)^{-1} dp \\ &= 2 \int_{p_-}^{p_+} \frac{dp}{\sqrt{(U^+ - E)(E - U^-)}}. \end{aligned} \quad (42)$$

From the explicit form of the potential curves we find the period in terms of an elliptic integral as

$$\begin{aligned} T(E) &= \frac{2\sqrt{2}}{v\sqrt{p_+ - p_0}} \int_0^{\frac{\pi}{2}} \frac{d\theta}{\sqrt{1 - \frac{p_+ - p_-}{p_+ - p_0} \sin^2 \theta}} \\ &= \frac{2\sqrt{2}}{v\sqrt{p_+ - p_0}} K\left(\frac{p_+ - p_-}{p_+ - p_0}\right), \end{aligned} \quad (43)$$

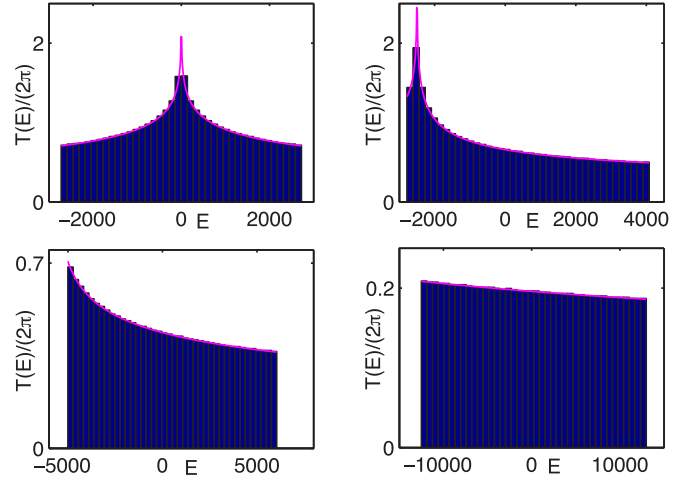


FIG. 9. (Color online) Density of states  $\frac{dn}{dE}$  for the many-particle system in comparison with the mean-field periods for  $v = 1$  and different values of  $\epsilon$ . The many-particle density of states is approximated by the normalized histogram of the energies, for  $N = 10000$  particles. The mean-field result is depicted by the solid magenta line. The values of  $\epsilon$  are  $\epsilon = 0, 1, 2, 5$  from top left to bottom right.

where  $p_0$  is the third root of the polynomial (35), and  $K$  denotes the complete elliptic integral of the first kind. The period diverges at the classical turning point, which can be seen as follows. At the value  $E = -\frac{\epsilon}{2}$ , corresponding to the orbit passing through the tip of the teardrop, the polynomial (35) can be explicitly factorized as

$$P(E = -\frac{\epsilon}{2}) = (p + \frac{1}{2})^2 (2v^2 p - v^2 + \epsilon^2). \quad (44)$$

That is, in the subcritical case  $|\epsilon| < \sqrt{2}|v|$ , where the fixed point at the tip corresponds to a saddle point, we have  $p_0 = p_- = -\frac{1}{2}$ , and  $p_+ = \frac{1}{2} - \frac{\epsilon^2}{2v^2}$ , that is, we have  $T(E) \propto K(1)$ , which diverges. For supercritical values, on the other hand, where the fixed point corresponds to the minimum of the energy, we have  $p_- = p_+ = -\frac{1}{2}$ , and  $p_0 = \frac{1}{2} - \frac{\epsilon^2}{2v^2} < -\frac{1}{2}$ . Thus, the period has the finite value of  $\frac{\sqrt{2\pi}}{\sqrt{\frac{\epsilon^2}{2} - v^2}}$  in this case.

Figure 9 depicts the normalized histogram of many-particle eigenvalues for a large particle number of  $N = 10000$  in comparison to the mean-field periods (divided by  $2\pi$ ), which are given by the analytical expression (43). Note that the mean-field energies are rescaled with respect to the many-particle energies by  $\eta$ . An excellent agreement between the analytical expression and the many-particle density of states is observed. In particular the accumulation of states around the classical saddle point for values of  $\epsilon$  below the critical value is nicely recovered in the many-particle histogram. Since the period of the orbit through the saddle point is infinite, the accumulation of many-particle eigenstates at this point leads to an actual divergence in the limit  $N \rightarrow \infty$ , which can be connected to a quantum phase transition [8].

We can also obtain an approximation for the components of the eigenvectors in the standard basis of  $\hat{K}_z$ , via a simple WKB ansatz. In the classically allowed region (between the two turning points) we make the ansatz

$$\psi(p) = \sqrt{w_{cl}(p)} (A_+ e^{i\eta S(p)} + A_- e^{-i\eta S(p)}), \quad (45)$$

where  $w_{\text{cl}}$  denotes the classical probability distribution

$$|w_{\text{cl}}(p)| = \frac{1}{2T} \left( \frac{\partial H}{\partial q} \right)^{-1} = \frac{1}{2T \sqrt{\frac{v^2}{4}(1-2p)(1+2p)^2 - (E - \epsilon p)^2}}, \quad (46)$$

and the action  $S(p)$  is given by

$$S(p) = \begin{cases} \pi(p - p_-) - \tilde{S}(p), & p_{\pm} \text{ on } U_- \\ \pi(\frac{1}{2} - p) - \tilde{S}(p), & p_- \text{ on } U_-, p_+ \text{ on } U_+ \\ \pi(\frac{1}{2} + p) - \tilde{S}(p), & p_- \text{ on } U_+, p_+ \text{ on } U_- \\ -\pi + \tilde{S}(p), & p_{\pm} \text{ on } U_+ \end{cases}, \quad (47)$$

with

$$\tilde{S}(p) = \int_{p_-}^p q(p) dp. \quad (48)$$

In the forbidden region the WKB ansatz reduces to the single exponential decaying solution

$$|\psi_{\text{cl}}(p)|^2 = \frac{1}{2} \left| \omega_{\text{cl}}(p) \exp\left(-\frac{2i}{\eta} S(p)\right) \right|^2, \quad (49)$$

with

$$S(p) = \begin{cases} \mp \int_p^{p_-} q(p) dp, & p < p_-, p_- \text{ on } U_{\pm} \\ \mp \int_{p_+}^p q(p) dp, & p > p_+, p_+ \text{ on } U_{\pm} \end{cases}. \quad (50)$$

The matching conditions at the boundary then impose the quantization condition (33) and the absolute value of the WKB wave function in the classically allowed region becomes

$$|\psi_{\text{cl}}(p)|^2 = 2|w_{\text{cl}}(p)| \cos^2\left(\eta^{-1} S(p) - \frac{\pi}{4}\right). \quad (51)$$

While this expression appears to depend on the continuous variable  $p$ , for finite values of  $\eta$   $p$  can only take on discrete values, due to the periodicity of its conjugate variable  $q$ , to which it can be related via a discrete Fourier transform. We thus have the semiclassical approximation

$$|\Psi_n\rangle = \sum_{m=-\frac{N}{4}:1:\frac{N}{4}} \psi_{\text{cl}}(\eta m) |m\rangle, \quad (52)$$

where  $|m\rangle$  denotes the eigenvectors of  $\hat{K}_z$ , that is, the states with  $2m + \frac{N}{2}$  atoms and  $\frac{N}{4} - m$  molecules. Figure 10 depicts examples of the exact many-particle eigenvectors in comparison to the semiclassical approximation (normalized to fit the central maximum). As expected, the semiclassical approximation breaks down in the vicinity of the turning points, but approximates the many-particle wave functions well for other values.

## VI. SUMMARY AND OUTLOOK

While the role of many-particle effects in cold atom systems is crucial, in large realistic systems the mean-field approximation is often all that is accessible. Thus, the possibility to recover many-particle features from the mean-field description is an important addition to the theoretical toolbox for cold atoms. Here we have demonstrated that semiclassical methods can be modified to deduce

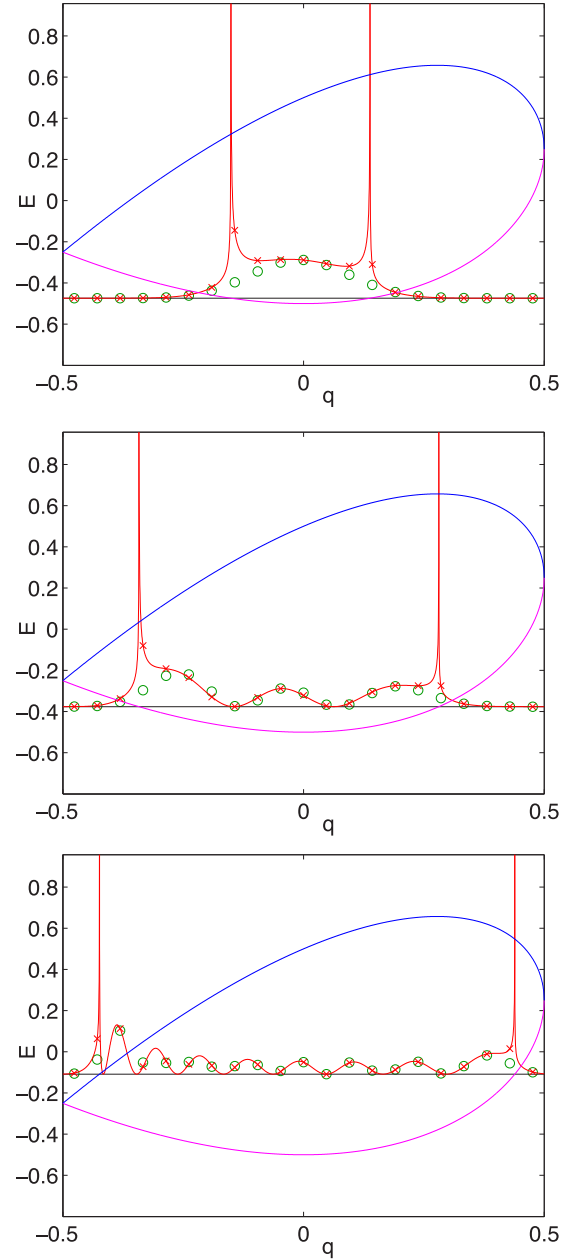


FIG. 10. (Color online) Exact  $n$ th many-particle eigenvectors (green circles) with the WKB wave function (red) for  $N = 40$ ,  $\epsilon = 0.5$ , and  $v = 1$  for  $n = 1$  (top),  $n = 3$  (middle), and  $n = 10$  (bottom). The red crosses indicate the semiclassical wave function (52). The solid red line, indicating the continuous semiclassical wave function according to Eq. (51), is added to guide the eye.

many-particle properties for atom-molecule conversion systems from the mean-field dynamics alone. We have considered the eigenvalues and eigenvectors here; an extension to dynamical properties via semiclassical propagators is an important topic for future investigations. A nontrivial issue is the generalization to more realistic models with many modes for both atoms and molecules. Progress has been made in this direction for cold atomic systems without atom-molecule conversion in [4,6]. The combination with the results obtained here suggests that this goal is not out of reach. An obstacle



for the application of some semiclassical techniques in the absence of a well-defined set of condensed states that coincide with coherent states of the deformed  $\text{su}(m)$  algebra for atom-molecule conversion systems. There have been proposals for coherent states in [14,30], however they do not fulfill all the properties that one relies on in the case of cold atoms in  $m$  mode systems when employing  $\text{su}(m)$  coherent states [31]. The connection between coherent states and projective manifolds [32] for  $\text{su}(m)$  systems might lead a way forward.

## ACKNOWLEDGMENTS

The authors thank Hans Jürgen Korsch for valuable comments on the manuscript. E.M.G. acknowledges support via an Imperial College Junior Research Fellowship; a L'Oréal-UNESCO for Women in Science UK and Ireland Fellowship, and a Royal Society University Research Fellowship (Grant. No. UF130339). A.R. acknowledges support from the Engineering and Physical Sciences Research Council via the Doctoral Research Allocation Grant No. EP/K502856/1.

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