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Bistability and quantum fluctuations in coherent photoassociation of a Bose-Einstein condensate

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We show that there exists bistability in coherent photoassociation of a Bose-Einstein condensate and investigate the corresponding quantum fluctuations. The simple analytical expressions obtained demonstrate clearly how to sweep adiabatically the frequency of the driving laser to convert a condensate of atoms into a condensate of molecules in an optimum and deterministic way.

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Over the last few years, there has been considerable effort devoted to the photoassociation of a Bose-Einstein condensate which occurs when an atom pair interacts with a photon, thereby making a transition from the two-atom continuum to a bound state of the molecule [1–5,7–11]. Quantizing the molecular dissociation continuum allows one to describe such free-bound transitions using standard few-level quantum optics [1–5,7–9]. One of the most important findings is the observation [1–5] that it is the Bose enhancement that ultimately facilitates coherent transients such as Rabi flopping, adiabatic following, and stimulated Raman adiabatic passage in photoassociation of a condensate. Based on a two-mode model for coherent photoassociation of a Bose-Einstein condensate, Javanainen and Mackie [3] have found by numerical calculations that for a large positive detuning the ground state of the two-mode model is the state with all atoms while for a large negative detuning it is the state with all molecules. Therefore they have put forward a photoassociation scheme that starting with all atoms and a large positive detuning, one sweeps the detuning slowly from a large positive detuning to a large negative detuning so that the system will move adiabatically from the state with all atoms to the state with all molecules. Such a scheme has subsequently been generalized to a Raman-type three-mode situation [4–6].

In this paper, we shall show that there exists in fact bistability in coherent photoassociation of a Bose-Einstein condensate based on the same two-mode model proposed by Javanainen and Mackie [3], and investigate the corresponding quantum fluctuations of atom, molecule numbers, and a certain phase difference at the bistable states. We shall derive the simple analytical expressions of the bistable states and the corresponding quantum fluctuations. These expressions clearly demonstrate how to sweep adiabatically the frequency of the driving laser to convert a condensate of atoms into a condensate of molecules in an optimum and deterministic way. In particular, to achieve efficient photoassociation, one needs to sweep the frequency of the drive laser from a large positive detuning to a large negative detuning in certain circumstance while the frequency sweeping should be in a reverse direction in another circumstance. Besides, the detuning in both circumstances should be within certain range.

We consider the following two-mode model for coherent photoassociation of a Bose-Einstein condensate [3,5] ($\hbar=1$):

$$H=-\frac{\delta}{2}a^{\dagger}a-\frac{\kappa}{2}(aab^{\dagger}+ba^{\dagger}a^{\dagger}), \tag{1}$$

where a and b are annihilation operators for atom (with a zero momentum) and molecule (with a momentum $\mathbf{q}$), respectively, κ is the photoassociation (and photodissociation) coupling parameter and without any loss of generality, we have chosen κ to be real and non-negative, the real parameter $\delta=\delta_0+q^2/2m$ is the detuning corrected for the photon recoil energy of the molecule, and the detuning $\delta_0>0$ corresponds to tuning of the laser by the energy $h\delta_0$ above the photassociation threshold. Obviously, there exists a conserved quantity $a^{\dagger}a+2b^{\dagger}b=N$ for such a system. Here, N is the total atom number for a condensate of all atoms or twice the total molecule number for a condensate of all molecules.

It is pointed out that in the two-mode model considered here, atoms (molecules) described by creation operator $a^{\dagger}$ ($b^{\dagger}$) and annihilation operator a (b) are assumed to be in the same atomic (molecular) Bose-Einstein condensated state so that $a^{\dagger}$ ($b^{\dagger}$) creates an atom (molecule) whose spatial distribution is described by a macroscopic wave-function $\Psi_a(\mathbf{r})$ [$\Psi_m(\mathbf{r})$]. Here the macroscopic wave-functions $\Psi_a(\mathbf{r})$ and $\Psi_m(\mathbf{r})$ for the mean-field condensates can be modeled by a set of two coupled Gross-Pitaevskii nonlinear equations [6,14] which take the spatial variations and inter-atomic (-molecular) interactions into account. The spatial variations and particle interactions can be similarly discussed by numerically solving a set of two coupled Gross-Pitaevskii nonlinear equations which are identical in form to the first two equations in Eq. (5) of Ref. [6] except for taking their $\Omega=0$. Consequently, we shall here focus on the bistability and quantum fluctuation behaviors described by the model Hamiltonian (1).

The Heisenberg equations of motion for a and b are

$$\dot{a}=i\frac{\delta}{2}a+i\kappa a^{\dagger}b, \quad \dot{b}=i\frac{\kappa}{2}a^2, \tag{2}$$

which, after the replacement $a\rightarrow\alpha$, $b\rightarrow\beta$, become

$$\dot{\alpha}=i\frac{\delta}{2}\alpha+i\kappa\alpha^{\star}\beta, \quad \dot{\beta}=i\frac{\kappa}{2}\alpha^2, \tag{3}$$

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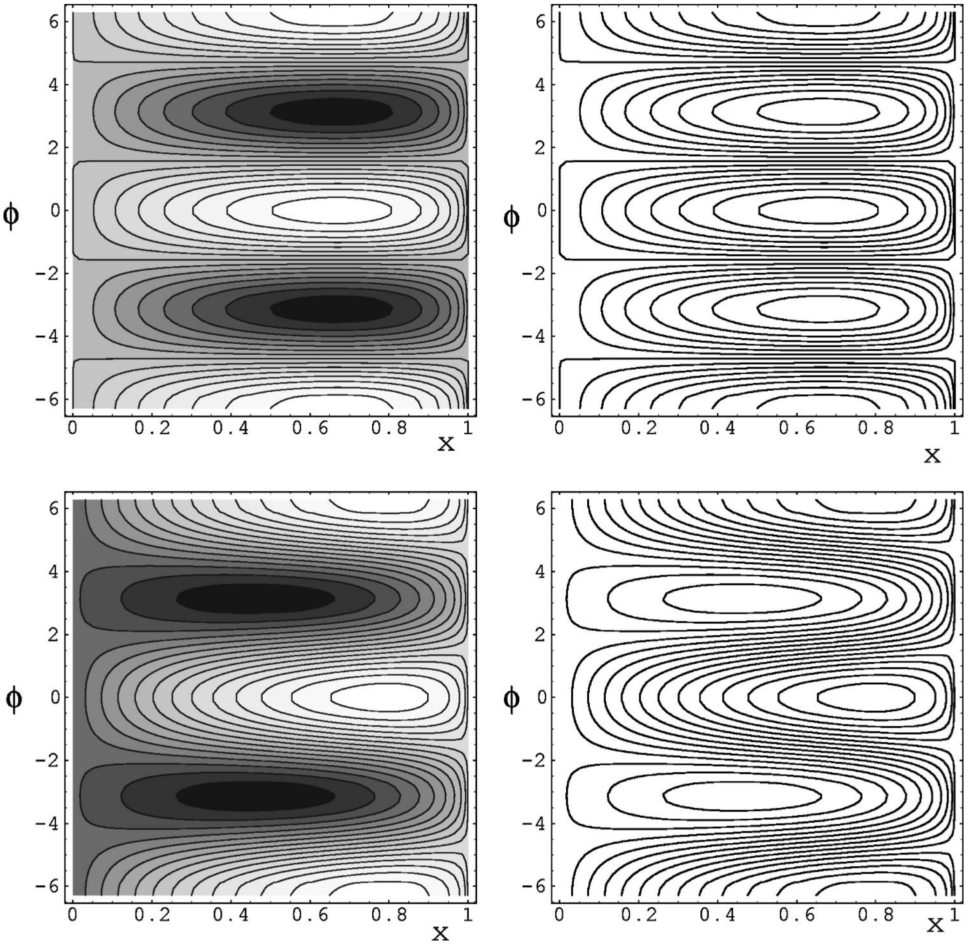

FIG. 1. The $\mathcal{H}$ contours in phase space of the scaled atom number $x=n/N$ (horizontal axis) and the phase difference ϕ (vertical axis). The scaled detuning $\overline{\delta}=0$ for the two top plots, and $\overline{\delta}=0.4$ for the two bottom plots. The plots on the left are the same as their (horizontally) right ones except that the left plots have contour shading while the right ones have not. The lighter contour shading represents a greater value of the $\mathcal{H}$ contour.

where $\alpha=|\alpha|e^{i\phi_\alpha}$ and $\beta=|\beta|e^{i\phi_\beta}$ are two complex numbers. Such replacement is the so-called semiclassical approach analogous to the Gross-Pitaevskii approximation used to describe an alkali condensate [4,12].

Let $n=|\alpha|^2$ and $\phi=2\phi_\alpha-\phi_\beta$, noting $2|\beta|^2=N-n$ and introducing the scaled time $\tau=\sqrt{2N}\kappa t$, scaled detuning $\overline{\delta}=\delta/\sqrt{2N}\kappa$, and scaled atom number $x=n/N$, we can from Eq. (3) obtain a couple of canonical Hamiltonian equations for the conjugate variables x and ϕ as follows:

$$\frac{dx}{d\tau}=-\frac{\partial\mathcal{H}}{\partial\phi}=x\sqrt{1-x}\sin\phi, \tag{4a}$$

$$\frac{d\phi}{d\tau}=\frac{\partial\mathcal{H}}{\partial x}=\overline{\delta}+\left[\sqrt{1-x}-\frac{x}{2\sqrt{1-x}}\right]\cos\phi, \tag{4b}$$

$$\mathcal{H}=\overline{\delta}x+x\sqrt{1-x}\cos\phi. \tag{5}$$

In general, the analytical solutions to Eq. (4) can be obtained and expressed in terms of elliptic functions [13]. However, the canonical Hamiltonian form of Eq. (4) allows us to grasp quickly and clearly the global behaviors of all the solutions by drawing phase diagrams, i.e., plotting the solution curves in the phase space spanned by the canonical conjugate variables x and ϕ. Obviously, the solution curves are nothing but the contours of the Hamiltonian (5), as shown in Fig. 1 for the scaled detuning $\overline{\delta}=0$, 0.4. We have plotted the phase diagrams in Fig. 1 for $0\leqslant x\leqslant 1$ and $-2\pi\leqslant\phi<2\pi$ for clarity although the phase space's actual range can be chosen as $0\leqslant\phi<2\pi$ and $0\leqslant x\leqslant 1$.

The fixed points (x_0,ϕ_0) correspond to steady-state solutions satisfying $(dx/d\tau,d\phi/d\tau)_{x=x_0,\phi=\phi_0}=0$. It readily shows that there exist two fixed points for the canonical Hamiltonian system (4), and their explicit analytical expressions are

$$\phi_0=0,\quad x_0=\frac{2}{9}\left[3-\overline{\delta}^2+\overline{\delta}\sqrt{\overline{\delta}^2+3}\right],\quad \overline{\delta}\geqslant-1, \tag{6a}$$

$$\phi_0=\pi,\quad x_0=\frac{2}{9}\left[3-\overline{\delta}^2-\overline{\delta}\sqrt{\overline{\delta}^2+3}\right],\quad \overline{\delta}\leqslant 1. \tag{6b}$$

In Fig. 2, we have plotted the diagram of the scaled atom number $x_0=n_0/N$ versus the scaled detuning $\overline{\delta}$ according to Eq. (6). The expressions (6) or the Fig. 2 clearly demonstrate how to vary the detuning δ or $\overline{\delta}$ so that the steady states of the system will follow the slowly varying detuning to move adiabatically from a condensate with all atoms $(x=1)$ to a condensate with all molecules $(x=0)$. It is worthwhile to mention two important points. First, just as is shown in Fig. 2 and Eq. (6), to achieve efficient photoassociation for the steady state with $\phi_0=0$, one needs to vary adiabatically the

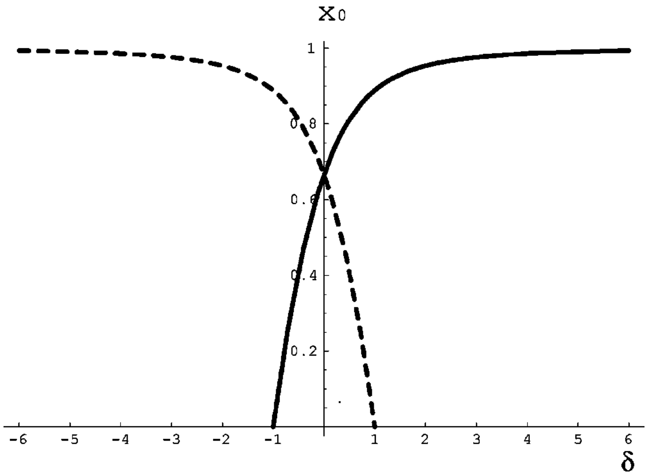

FIG. 2. Diagram of the scaled atom number $x_0 = n_0/N$ (vertical axis) at the fixed points versus the scaled detuning $\bar{\delta}$ (horizontal axis). The solid and dashed lines correspond to the fixed points at $\phi_0 = 0$ and $\phi_0 = \pi$, respectively.

detuning (by sweeping the frequency of the driven laser) from a high positive value $\bar{\delta}$ to a negative value just as mentioned by Javanainen and Mackie through numerical calculations [3]. However, a fact is that the detuning should vary in a reverse direction, i.e., from a high-negative value $\bar{\delta}$ to a positive value, for the steady state with $\phi_0 = \pi$. Second, there exists one and only one steady state if the scaled detuning satisfies $|\bar{\delta}| > 1$. To be more specific, the steady state with $\phi_0 = 0$ does not exist at all if $\bar{\delta} < -1$, while neither does the steady state with $\phi_0 = \pi$ if $\bar{\delta} > 1$. This fact carries the implication for the efficient photoassociation. For instance, when the system is initially in the steady state with $\phi_0 = 0$, if the detuning is swept from a high-positive value to a high-negative value so that $\bar{\delta} < -1$, the large-amplitude Rabi-type oscillations of coherent photoassociation and photodissociation will inevitably set in, which is obvious a detriment result that should be avoided in efficient photoassociation.

There occurs naturally the question whether the two steady states described by Eq. (6) are stable. A naive thought might be that the steady state with $\phi_0 = \pi$ is stable while another steady state is unstable because contours of the Hamiltonian (5) as shown in Fig. 1 display a hill (peaked at the fixed point with $\phi_0 = 0$) and valley (its lowest is the fixed point with $\phi_0 = \pi$) structure. However, as will be seen shortly, both steady states are in fact stable or neutral stable in more accurate terminology. To illustrate this point, substituting $\phi = \phi_0 + \delta\phi$ and $x = x_0 + \delta x$ into Eq. (4) and omitting those terms of the order greater than $O(\delta\phi, \delta x)$, we obtain the linearized equations as follows:

$$\frac{d}{d\tau}\delta x = x_0\sqrt{1-x_0}\cos\phi_0\,\delta\phi, \tag{7a}$$

$$\frac{d}{d\tau}\delta\phi = -\frac{4-3x_0}{4(1-x_0)^{3/2}}\cos\phi_0\,\delta x. \tag{7b}$$

It is then straightforward to see that both $\delta\phi$ and δx perform simple harmonic oscillations with the frequency $\omega = \sqrt{x_0(1-3x_0/4)/(1-x_0)}$ no matter whether $\phi_0 = 0$ or $\phi_0 = \pi$. Consequently, the two steady states described by Eq. (6) are indeed stable.

Now we are ready to investigate the quantum fluctuations of the atom number n (as well as the molecule number $=(N-n)/2$) and phase difference ϕ around the fixed points. One advantage of the Hamiltonian formalism (4) and (5) of the semiclassical approach is to provide a natural basis for describing quantum mechanically the atom number and phase statistics. We first substitute $n = n_0 + \eta$ (or $x = x_0 + N^{-1}\eta$ with $n_0 = Nx_0$) and $\phi = \phi_0 + \psi$ into the Hamiltonian (5) and expand it as the series of the variables η and ψ up to the order $O(\eta^2, \eta\psi, \psi^2)$ (see the Appendix for the derivation of such a series). Then by utilizing the standard quantization procedure [15,16] $n \to \hat{n} = n_0 + \hat{\eta}$ (or $x \to \hat{x} = x_0 + N^{-1}\hat{\eta}$) and $\phi \to \hat{\phi} = \phi_0 + \hat{\psi}$ with the commutative relation $[\hat{n}, \hat{\phi}] = i$ or $[\hat{\eta}, \hat{\psi}] = i$, it is now straightforward to obtain an operator-valued Hamiltonian $\hat{\mathcal{H}}$ which has the following form in the η representation $\hat{\eta} = \eta$ and $\hat{\psi} = -i\partial/\partial\eta$ (see the Appendix for the derivation of the following equation):

$$\hat{\mathcal{H}} \approx \mathcal{H}_0 - \frac{E_J}{2}\frac{\partial^2}{\partial\eta^2} + \frac{E_C}{2}\eta^2, \tag{8}$$

where $\mathcal{H}_0$ is a c number equal to $\mathcal{H}$ in Eq. (5) evaluated at the fixed points (x_0, ϕ_0), and

$$E_J = -\cos\phi_0 x_0\sqrt{1-x_0}, E_C = -\frac{\cos\phi_0(4-3x_0)}{4N^2(1-x_0)^{3/2}}. \tag{9}$$

Equation (8) for $\phi_0 = \pi$ is nothing but a simple harmonic-oscillator model. However, both E_J and E_C are negative for $\phi_0 = 0$. But this circumstance also corresponds to a simple harmonic oscillator model which can be imagined as a particle with negative mass moving in an upside down harmonic potential and hence also represents a stable simple harmonic oscillation in agreement with our semiclassical stability analysis in the last paragraph.

It is well known that the width of the probability density of a simple harmonic oscillator characterizes its position uncertainty. Consequently, the statistical deviation for the quantum fluctuation of the scaled atom number described by the simple harmonic-oscillator model (9) is easily shown to be $\Delta n = \Delta\eta = (E_J/E_C)^{1/4} = \sqrt{N}x_0^{1/4}(1-x_0)^{1/2}(1-3x_0/4)^{-1/4}$ when the harmonic oscillator is in its ground state. The statistical deviation $\Delta\phi = \Delta\psi$ can then be obtained by using the minimum uncertainty relation $\Delta\psi\Delta n = 1/2$ which is obtained by using the commutative relation $[\hat{n}, \hat{\phi}] = i$ and the fact that the ground state of a harmonic oscillator is a minimum uncertainty state. Consequently we finally obtain the results for the quantum fluctuations of the relative atom number and phase difference around the fixed points as follows:

$$\frac{\Delta n}{n_0}=\frac{(1-x_0)^{1/2}}{N^{1/2}x_0^{3/4}}\,\frac{1}{(1-3x_0/4)^{1/4}}\sim\frac{(1-x_0)^{1/2}}{N^{1/2}x_0^{3/4}}, \tag{10}$$

$$\Delta\phi=\frac{(1-3x_0/4)^{1/4}}{2N^{1/2}x_0^{1/4}(1-x_0)^{1/2}}\sim\frac{1}{2N^{1/2}x_0^{1/4}(1-x_0)^{1/2}}, \tag{11}$$

where the factors $(1-3x_0/4)^{-1/4}$ and $(1-3x_0/4)^{1/4}/2$ are of the order one throughout the interval $x_0\in[0,1]$ and hence have little effect on estimation of the quantum fluctuations. The above analytical expressions display that the quantum fluctuation of the relative atom number is at most the order $O(N^{-1/2})$ except for a very small regime near $x_0=0$. In addition, the quantum fluctuation of the phase difference is also of the order $O(N^{-1/2})$ except for two very small regimes near $x_0=0$ and $x_0=1$, respectively.

Let us discuss the impact of the quantum fluctuations on the scheme of photoassociation mentioned in the paragraph after Eq. (6). As we have mentioned in the last paragraph, the quantum fluctuation of the relative atom number is at most the order $O(N^{-1/2})$ except for a very small regime near $x_0=0$ where the quantum fluctuation of relative atom number behaves according to the scaling law $\Delta n/n_0\sim N^{-1/2}x_0^{-3/4}$. Therefore so long as $x_0\equiv n_0/N\gg N^{-2/3}$ (obtained from $\Delta n/n_0\ll 1$) is satisfied, quantum fluctuations would affect little on the scheme. Taking $N=10^6$, one finds that such a condition requires $n_0/N\gg 10^{-4}$, implying that the scheme is still suitable when nearly all atoms have photoassociated into molecules. Even for the moderate N such as $N=10^3$, such a condition $n_0/N\gg 1\%$ places not much restriction to the scheme in most of practical situations.

In summary, we have shown that there exists bistability in coherent photoassociation of a Bose-Einstein condensate based on a two-mode model, and have obtained the analytical expressions of the bistable steady states. It is interesting to note that the phenomenon of multiple solutions also exists in the four-wave mixing with matter waves in a Bose-Einstein condensate but only one of them is stable [17]. While in our case, both steady states are stable ones. We have shown that the two-mode model under the semiclassical approximation can be put into a couple of canonical Hamiltonian equations for the conjugate variables atom number and a phase difference. Such canonical Hamiltonian formalism not only permits one to understand the global behaviors of the whole solutions clearly but also offers a natural basis to study the quantum fluctuations of atom, molecule numbers, and the phase difference around the bistable states. In this way, we have obtained the analytical expressions describing such quantum fluctuations.

Besides, we have based our above-mentioned results to investigate the scheme of photoassociation through sweeping adiabatically the frequency of the driving laser originally proposed by Javanainen and Mackie and studied by them through numerical calculations [3]. In this regard, the analytical expressions (6) of the bistable steady states appear to be particularly useful because they demonstrate clearly how to sweep adiabatically the frequency of the driving laser to convert a condensate of atoms into a condensate of molecules in an optimum and deterministic way. They have also revealed two features concerning the efficient photoassociation: (1) one needs to sweep the frequency of the drive laser from a large positive detuning to a large negative detuning in one circumstance while the frequency sweeping should be in a reverse direction in another circumstance; and (2) the detuning should not vary outside a certain range explicitly given in Eq. (6). In addition, the analytical expression (10) describing the quantum fluctuation of atom and molecule numbers implies that the scheme should be suitable so long as the remaining atom number satisfies $n_0/N\gg N^{-2/3}$. In other words, we have shown that the scheme is basically immune from quantum fluctuations at least in the thermodynamic limit. Before ending this paper, we would like to mention that the solutions $\phi=\pm\pi/2$ and $x(\tau)=1-\tanh^2(\tau/2)$ to Eq. (4) are unsuitable for an efficient photoassociation because it can be shown that even an infinitesimal perturbation would cause them to become solutions describing large oscillations around one of the two fixed points, which can also readily be understood by looking at the solution curves in Fig. 1.

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APPENDIX

In this appendix, we present the detailed derivation of Eq. (8) in the main text. We first substitute $n=n_0+\eta$ (or $x=x_0+N^{-1}\eta$ with $n_0=Nx_0$) and $\phi=\phi_0+\psi$ into the Hamiltonian (5) and expand it as the series of the variables η and ψ up to the order $O(\eta^2,\eta\psi,\psi^2)$ as follows:

$$\begin{aligned}\mathcal{H}=\mathcal{H}_0&+\left(\frac{\partial\mathcal{H}}{\partial x}\right)_0(x-x_0)+\left(\frac{\partial\mathcal{H}}{\partial\phi}\right)_0(\phi-\phi_0)\\&+\frac{1}{2}\left(\frac{\partial^2\mathcal{H}}{\partial x^2}\right)_0(x-x_0)^2+\frac{1}{2}\left(\frac{\partial^2\mathcal{H}}{\partial\phi^2}\right)_0(\phi-\phi_0)^2\\&+\left(\frac{\partial^2\mathcal{H}}{\partial\phi\partial x}\right)_0(\phi-\phi_0)(x-x_0)+O(\eta^2,\eta\psi,\psi^2),\end{aligned} \tag{A1}$$

where $\mathcal{H}_0$, $(\partial\mathcal{H}/\partial x)_0$, etc., are $\mathcal{H}$, $\partial\mathcal{H}/\partial x$, etc., evaluated at the fixed points $(x,\phi)=(x_0,\phi_0)$. Using the explicit expression of Hamiltonian (5), noting $\sin\phi_0=0$ and that the fixed points (x_0,ϕ_0) correspond to steady-state solutions satisfying $(dx/d\tau, d\phi/d\tau)_{x=x_0,\phi=\phi_0}=0$ or $(\partial\mathcal{H}/\partial x)_0=(\partial\mathcal{H}/\partial\phi)_0=0$ according to Eq. (4), we can readily obtain $(\partial^2\mathcal{H}/\partial\phi\partial x)_0=0$, and

$$\mathcal{H}=\mathcal{H}_0+\frac{E_J}{2}\psi^2+\frac{E_C}{2}\eta^2+O(\eta^2,\eta\psi,\psi^2) \tag{A2}$$

with

$$E_J=\left(\frac{\partial^2\mathcal{H}}{\partial\phi^2}\right)_0=-\cos\phi_0 x_0\sqrt{1-x_0}, \tag{A3a}$$

$$E_C=\frac{1}{N^2}\left(\frac{\partial^2\mathcal{H}}{\partial x^2}\right)_0=-\frac{\cos\phi_0(4-3x_0)}{4N^2(1-x_0)^{3/2}}. \tag{A3b}$$

Then by utilizing the standard quantization procedure $n\rightarrow\hat{n}=n_0+\hat{\eta}$ (or $x\rightarrow\hat{x}=x_0+N^{-1}\hat{\eta}$) and $\phi\rightarrow\hat{\phi}=\phi_0+\hat{\psi}$ with the commutative relation $[\hat{n},\hat{\phi}]=i$ or $[\hat{\eta},\hat{\psi}]=i$, it is now straightforward to obtain an operator-valued Hamiltonian $\hat{\mathcal{H}}$ which has the form of Eq. (5) in the main text in the η representation $\hat{\eta}=\eta$ and $\hat{\psi}=-i\partial/\partial\eta$.

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