Higher energy collective excitations in trapped Bose condensates

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Abstract: We investigate theoretically the collective excitations of trapped Bose condensates with energies of the order of the chemical potential of the system. For the MIT sodium Bose condensate in a Cloverleaf trap, we find interesting level crossing behavior for high energy excitations and calculate the spatial magnetic dipole moments for selective creation of condensate excitations.

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The experimental realization of Bose–Einstein condensation (BEC) in trapped alkali atoms[1−3] has generated great interest in studying the properties of these confined weakly interacting quantum gases. Tremendous progress has been made in the past two years: many single particle properties of trapped condensates have been measured; direct nondestructive optical imaging techniques have been developed[4−5]; and several of the low energy collective excitation modes have been detected[6−8]. Recently, the macroscopic coherence properties of the condensate were displayed in a spectacular fashion by the demonstration of the interference of two condensates[9], and by the suppression of condensate collisional losses from inelastic collisions[10] due to multi-particle correlations. Rudimentary atom lasers with pulsed output couplers have also recently been deveoped[9,11], and the zero-sound velocity of the condensate has been measured[12].

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The theoretical description of these experiments has also been an active field. Among the most intensively studied properties are the low energy collective excitations of trapped condensates. In the low temperature limit, the pre-existing Bogoliubov Hartree (BH) theory has been widely and successfully applied. This theory describes condensate excitations in terms of nominally non-interacting quasi-particles. The Bogoliubov-de Gennes equations for quasi-particles have also been studied by several groups[13,14]. An (analytic) asymptotic expression for excitation eigenfrequencies, valid in the Thomas-Fermi/hydrodynamic limit, was first presented by S. Stringari[15]. A variational approach was developed by A. Fetter[16], and a dynamical variational approach was applied by V. M. Pérez-García, *et al*[17]. More recent studies in this area are listed in Ref. $18-23$. These investigations describe the condensate within a mean-field approximation with excitations corresponding to the poles of the single particle Green's function. The calculated mode structure and eigenfrequencies for low energy collective excitations are in good agreement with experimental results to date, leading to confidence in this application of the mean field BH theory. However, recent work indicates that agreement between experiment[8] and theory[24–26] may be difficult to achieve at finite temperatures and for high energy excitations.

In particular, recent studies[26,27] by two of us and co-workers, indicate that quasi-particles (i.e. collective excitations) display interesting dynamics. A careful numerical study of the dependence of the excitation frequencies on the total number of condensate atoms at zero temperature[27] (i.e. the interaction strength of the condensate), found complicated level crossings and avoided crossings[26]. Similar behavior for high energy excitations was also recently predicted by Fliesser, et. al.[28,29], where they studied the classical dynamics of the condensate quasi-particles using a semiclassical approach. They found that for non-isotropic harmonic traps, quasi-particles can be chaotic when their excitation energy is of the order of the system's chemical potential. It will, of course, be important to study quasi-particle dynamics quantum mechanically to confirm the semiclassical studies. In this paper, we further such investigation of high energy collective excitations. We present new calculations, for the MIT sodium condensate in a Cloverleaf trap[7], of the symmetry properties of the quasi-particle level structure, and of selective quasi-particle excitation using spatial magnetic resonance[30].

We begin with a brief overview of the mean field BH theory of trapped Bose condensates at zero temperature.

The second quantized Hamiltonian for a system of N spinless bosonic atoms trapped in a potential $V_t(\vec{r})$ is given by

$$\mathcal{H} = \int d\vec{r}\,\hat{\Psi}^\dagger(\vec{r})\left[-\frac{\hbar^2}{2M}\nabla^2 + V_t(\vec{r}) - \mu\right]\hat{\Psi}(\vec{r}) + \frac{u_0}{2}\int d\vec{r}\,\hat{\Psi}^\dagger(\vec{r})\hat{\Psi}^\dagger(\vec{r})\hat{\Psi}(\vec{r})\hat{\Psi}(\vec{r}), \quad (1)$$

where $\hat{\Psi}(\vec{r})$ and $\hat{\Psi}^\dagger(\vec{r})$ are atomic (bosonic) annihilation and creation fields, $u_0 = 4\pi\hbar^2 a_{\rm sc}/M$, with M being the atomic mass, and $a_{\rm sc}$ is the scattering length of the atom-atom interaction. The chemical potential μ is introduced to guarantee conservation of the average of the total number of atoms $\hat{N} = \int d\vec{r}\,\hat{\Psi}^\dagger(\vec{r})\hat{\Psi}(\vec{r})$. The mean field BH theory describes the single particle excitations of the system in terms of non-interacting quasi-particles, thus casting the Hamiltonian (1) into the form

$$\mathcal{H} \to \sum_{k\neq 0} \hbar\tilde{\omega}_k \tilde{g}_k^\dagger \tilde{g}_k + (k=0 \text{ zero mode part } \cdots), \quad (2)$$

where $\tilde{g}_k^\dagger$ ($\tilde{g}_k$) are the quasi-particle creation (annihilation) operators that satisfy the standard bosonic commutation relations and the quasi-particle index, $k = 0, 1, 2, \ldots$, labels the positive eigenfrequencies $\tilde{\omega}_k$ arranged in ascending order. For $k = 0$, the system has a zero mode related to the phase of the condensate[31].

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At $T = 0$, the the Bogoliubov approximation starts with the assumption

$$\hat{\Psi}(\vec{r}) = \sqrt{N}\psi_0(\vec{r}) + \delta\hat{\Psi}(\vec{r}), \tag{3}$$

where the c-number condensate wave function $\psi_0(\vec{r})$ is assumed to be real without loss of generality, and is normalized according to $\int d\vec{r}|\psi_0(\vec{r})|^2 = 1$. $\delta\hat{\Psi}(\vec{r})$ represents the contributions of quantum fluctuations, and fulfills the same standard bosonic commutation relations as $\hat{\Psi}(\vec{r})$. We substitute Eq. (3) into Eq. (1) and neglect both 3-rd and 4-th order fluctuation terms. Linear fluctuation terms vanish provided $\psi_0(\vec{r})$ satisfies the nonlinear Schrödinger equation (NLSE), i.e.

$$[\mathcal{L} + u_0\rho_0]\,\psi_0(\vec{r}) = 0, \tag{4}$$

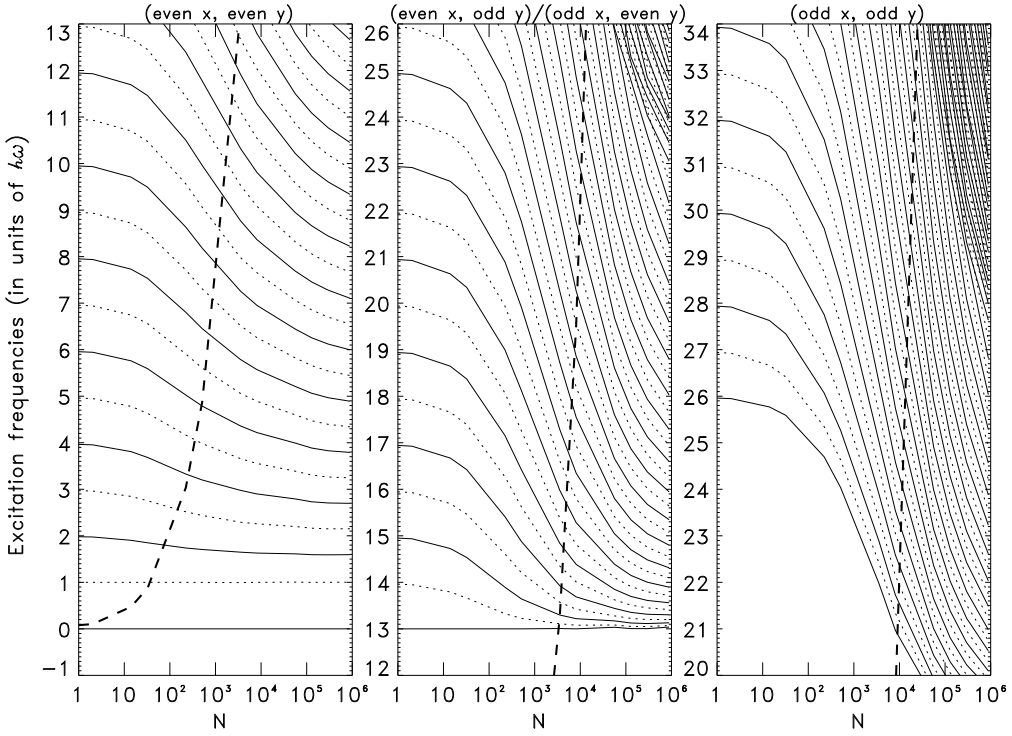

Fig. 1. The calculated dependence of quasi-particle excitation frequencies on the number of condensed sodium atoms N, for the MIT Cloverleaf trap. The three separate panels are for the 4 separate parity sectors in x and y coordinates respectively: the first panel shows (even x, even y), (note $\tilde{\omega}_k$ starts from 0 in the low N limit); the second panel shows (even x, odd y) [which is the same as the (odd x, even y) sector] ($\tilde{\omega}_k$ starts from $\omega_x = 13\omega$ in the low N limit); and the third panel shows (odd x, odd y) ($\tilde{\omega}_k$ starts from $\omega_x + \omega_y = 26\omega$ in the low N limit). The even z parity states are plotted with solid lines while the odd parity z states are plotted with thin dashed lines. The thick dashed line denotes the chemical potential.

where we have defined $\mathcal{L} \equiv -\frac{\hbar^2\nabla^2}{2M} + V_{\rm t}(\vec{r}) - \mu$, and the condensate density $\rho_0(\vec{r}) = N|\psi_0(\vec{r})|^2$. The resulting linearized Hamiltonian is then quadratic in $\delta\hat{\Psi}$ and $\delta\hat{\Psi}^\dagger$, and can be diagonalized by the quasi-particle annihilation operator

$$\tilde{g}_k = \int d\vec{r}[U_k(\vec{r})\delta\hat{\Psi}(\vec{r}) + V_k(\vec{r})\delta\hat{\Psi}^\dagger(\vec{r})], \tag{5}$$

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and its Hermitian conjugate, a quasi-particle creation operator $\tilde{g}_k^\dagger$. $U_k(\vec{r})$ and $V_k(\vec{r})$ are the mode functions of the quasi-particles, and must be calculated for particular traps and condensates. To determine the functions $U_k(\vec{r})$ and $V_k(\vec{r})$ (for $k \neq 0$) we solve $[\tilde{g}_k, \mathcal{H}] = \hbar\tilde{\omega}_k \tilde{g}_k$, which gives the following coupled Bogoliubov-de Gennes equations:

$$\begin{aligned}
&[\mathcal{L} + 2u_0\rho_0(\vec{r})]\, U_k(\vec{r}) - u_0\Delta_0^*(\vec{r})V_k(\vec{r}) = \hbar\tilde{\omega}_k U_k(\vec{r}),\\
&[\mathcal{L} + 2u_0\rho_0(\vec{r})]\, V_k(\vec{r}) - u_0\Delta_0(\vec{r})U_k(\vec{r}) = -\hbar\tilde{\omega}_k V_k(\vec{r}),
\end{aligned} \tag{6}$$

where $\Delta_0(\vec{r}) = N\psi_0^2(\vec{r})$. The mode functions obey the standard *orthonormality* condition[21]. The above Eqs. (4) and (6) may be solved for the condensate wavefunction $\psi_0(\vec{r})$ and the properties of quasi-particle excitations[26,27]. The details of our numerical approach are described in Ref. 26. Here we present new calculations for the MIT Cloverleaf trap[7] with $(\omega_x : \omega_y : \omega_z) = (13 : 13 : 1)(2\pi)19.28(\mathrm{Hz})$, the scattering length $a_{\mathrm{sc}} = 2.7$ (nm) for the sodium atom (the actual hyperfine state of the condensed atoms).

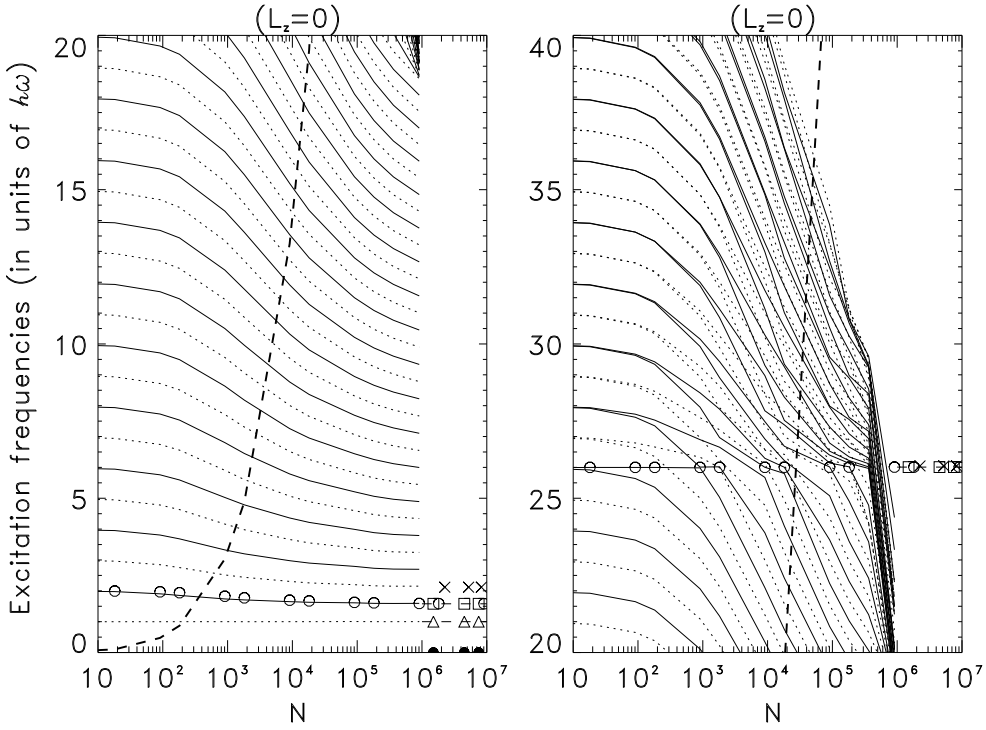

Fig. 2. The same calculations as in Fig. 1, now displaying the quasi-particle level structure for $L_z = 0$ excitations [a subset of the (even x, even y) parity sector shown in Fig. 1]. The open circles denote two calculated shape oscillation modes[17]. The high N, or asymptotic, limit of these two modes corresponds well with shapeoscillations observed in the MIT experiment[7]. The dashed line in the asymptotic limit, $N = 10^5 - 10^6$, are results based on Ref. 15. The filled circles, triangles, squares, and crosses denote, respectively, the modes labelled $n = 0, 1, 2, 3$ in Ref. 22.

Figs. 1 and 2 show the calculated dependence of the quasi-particle excitation frequencies on the number of Bose condensed sodium atoms. Fig. 1 displays the quasi-particle level structure in terms of spatial parity of the Cartesian coordinates in the laboratory reference frame. Note that this quasi-particle level structure segregates into three energy bands or families, with the (even x, even y) parity sector having the lowest energy quasi-particles and the (odd x, odd y) sector having the highest energy quasi-particles. Note also that the density of states increases rapidly for high energy excitations

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as N increases, i.e. as the mean field interactions grow. In Fig. 2 the N-dependence of the quasi-particle level structure is plotted for $L_z = 0$ excitations only, i.e. for excitations with no axial angular momentum. This figure shows the correspondence between two shape oscillations recently observed in the MIT BEC experiment[7], which operates in the high atom number limit ($N \approx 10^6$), and the $\tilde{\omega}_k = 2$ and $\tilde{\omega}_k = 26$ quasi-particle states in the low density limit. Note that level crossings become common for higher energy L_z=0 quasi-particles when the excitation energy is of the order of the system's chemical potential. It is worth emphasizing that the Eq. (6) is in fact a set of linear equations, and the observed complicated level repulsion behavior is not due to a simple nonlinear coupling between different quasiparticle modes.

Next, we discuss the technique of *spatial magnetic resonance* (SMR) recently analyzed by two of us for the selective creation and manipulation of quasi-particles[30]. The physics of SMR is straightforward and may be thought of as an optimized variation of the trap potential (or other applied magnetic fields). The variation is optimized to excite the condensate into higher quasi-particle states with a desired spatial symmetry while minimizing the perturbation of the trap potential, thus reducing the excitation of unwanted modes. In contrast, simple resonant variations of the trap potential will not be generally efficient at exciting high energy quasi-particles; in addition, such non-optimal trap potential variations will significantly perturb the condensate during application.

To illustrate the effectiveness of SMR, consider a very simple example of two quasi-particle states inside a one-dimensional trap. The lower energy quasi-particle state i (e.g. the condensate) is assumed to be spatially symmetric (an even function of spatial coordinate x in a one-dimensional symmetric trap), and the higher energy quasi-particle state f is assumed to be spatially antisymmetric (an odd function of x). The two trap state wavefunctions $\psi_i(\vec{r})$ and $\psi_f(\vec{r})$ describe the spatial extent of the respective quasi-particles; while the internal spin state $|\mathrm{IN}\rangle$, which describes the ensemble magnetic dipole moment of the atomic cloud, remains the same for both trapped states (in order for atoms to remain trapped). We introduce a time and space dependent magnetic field $\vec{B}_{\mathrm{SMR}}(\vec{r},t) = \hat{e}_B(\vec{r})B_{\mathrm{SMR}}(\vec{r})F(t)$, where $F(t) = \mathcal{F}(t)(e^{-i\omega_B t} + e^{i\omega_B t})$, $\mathcal{F}(t)$ is a slowly varying envelope function, and ω_B is close to resonance with the transition of the two quasi-particle states $\omega_f - \omega_i$. The unit vector $\hat{e}_B(\vec{r})$ denotes the direction of the time-dependent magnetic field. Then the ensemble magnetic dipole transition matrix element between the two quasi-particle states is

$$\begin{aligned} & -{}_i\langle\psi_i(\vec{r})|_i\langle\mathrm{IN}|\vec{\mu}_m\cdot\vec{B}_{\mathrm{SMR}}(\vec{r},t)|\mathrm{IN}\rangle_f|\psi_f(\vec{r})\rangle_f \\ &= -\mu_m\langle\psi_i(\vec{r})|\hat{e}_m(\vec{r})\cdot\hat{e}_B(\vec{r})B_{\mathrm{SMR}}(\vec{r})|\psi_f(\vec{r})\rangle F(t) \\ &\approx -\mu_m\langle\psi_i(\vec{r})|B_{\mathrm{SMR}}(\vec{r})|\psi_f(\vec{r})\rangle F(t), \end{aligned} \tag{7}$$

where the magnetic dipole moment of each atom is $\vec{\mu}_m = \mu_m\hat{e}_z(\vec{r})$, and we have assumed that the strong trapping field completely spin polarizes the atoms and is pointing along the z-axis[20]. Therefore the transition matrix element is a product of two parts: an internal part (a constant) due to the permanent magnetic moment $\vec{\mu}_m$ of the atoms; and a spatial part, which is the magnetic dipole transition analog of the Franck-Condon factor in electric dipole transitions in diatomic molecules. Now if $B_{\mathrm{SMR}}(\vec{r})$ is spatially symmetric, as in a simple trap potential variation, then the transition matrix element is zero when the initial and final quasi-particle states have opposite spatial parity. As long as $B_{\mathrm{SMR}}(\vec{r})$ has some spatial asymmetry, however, the matrix element is non-zero. For optimal SMR in this simple example, $B_{\mathrm{SMR}}(\vec{r})$ should be antisymmetric.

The SMR interaction can be incorporated into the BH theory[20] by the term

$$\mathcal{H}_{\mathrm{SMR}} = -\int d\vec{r}\,\hat{\Psi}^\dagger(\vec{r})\vec{\mu}_m\cdot\vec{B}_{\mathrm{SMR}}(\vec{r},t)\hat{\Psi}(\vec{r}), \tag{8}$$

in the Hamiltonian [Eq. (1)]. Expressed in terms of quasi-particles [see Eq. (5)], it takes the following form

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$$\mathcal{H}_{\rm SMR} = \mathcal{F}(t) \sum_{k,k'=0}^{\infty} \left[(\hbar u_{kk'} + \hbar v_{k'k}) \tilde{g}_k^\dagger \tilde{g}_{k'} - \hbar \gamma_{k'k}^* \tilde{g}_k \tilde{g}_{k'} - \hbar \gamma_{kk'} \tilde{g}_k^\dagger \tilde{g}_{k'}^\dagger \right], \tag{9}$$

where we have neglected a constant term, and defined the SMR coupling constants $\hbar u_{kk'} = -\mu_m \int d\vec{r} U_k(\vec{r}) U_{k'}^*(\vec{r}) B_{\rm SMR}(\vec{r})$ (and similarly for $\hbar v_{kk'}$ with V_k replacing U_k, etc.) and $\hbar \gamma_{kk'} = -\mu_m \int d\vec{r} U_k(\vec{r}) V_{k'}(\vec{r}) B_{\rm SMR}(\vec{r})$.

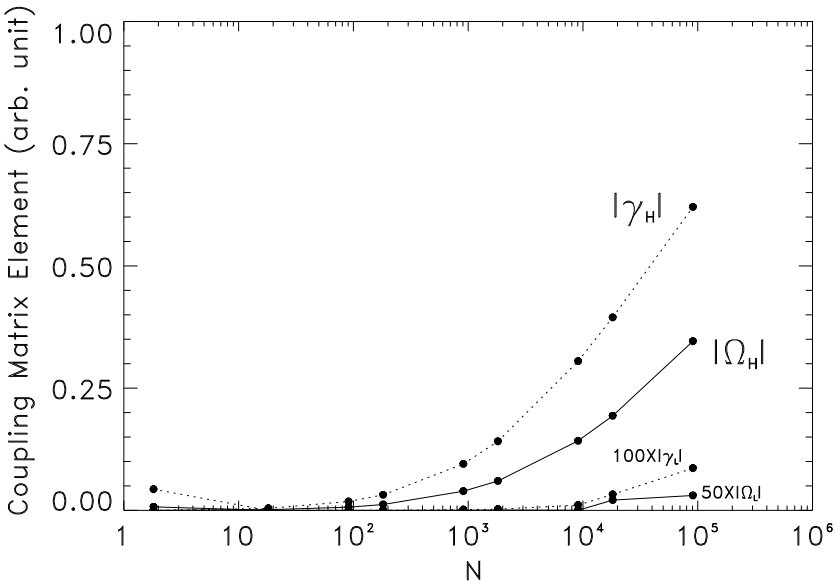

Fig. 3. Calculated SMR coupling constants for the two $L_z = 0$ quasi-particle modes that are degenerate at $\tilde{\omega}_k = 26$ when $N = 1$. These two modes are denoted as 'H' (for higher energy, this is the shape oscillation mode, see Fig. 2) and 'L' (for lower energy) with $\Omega_k = u_{0k} + v_{0k}$ and $\gamma_k = \gamma_{0k} + \gamma_{k0}$. A simple, spatially uniform SMR magnetic field was assumed. The dots denote the numerically computed points. As one can see, the coupling to the lower energy mode 'L' is practically zero with this spatially uniform SMR field.

In principle, the SMR coupling constants can be tailored to achieve optimal control of the quasi-particle dynamics. For example, for a spherically symmetric trap, the (ground) condensate state is described by spherically symmetric functions $U_0(r)$ and $V_0(r)$. The excited state wavefunctions factor into radial parts, $U_{kLL_z}(r)$ and $V_{kLL_z}(r)$; and into angular parts, the spherical harmonics $Y_{LL_z}(\theta, \phi)$ that are eigenstates of the angular momentum $\hat{L}^2$ and its projection on the z-axis $\hat{L}_z$. (Here k is the quantum number for the radial direction.) If the applied SMR field is chosen to have $B_{\rm SMR}(\vec{r})$ proportional to a particular spherical harmonic $Y_{LL_z}(\theta, \phi)$, then only quasi-particle states with this particular spatial symmetry have non-zero SMR coupling matrix elements from the condensate. A similar argument applies for the radial dependence of $B_{\rm SMR}(\vec{r})$. So by selecting the spatial symmetries of the applied magnetic field we can control the induced dipole coupling given in Eq. (9), and selectively create either specific quasi-particles or a coherent superposition of quasi-particles. (Note that when the initial state is not spherically symmetric, the spatial symmetries of the optimal SMR field will not in general be the same as the final quasi-particle state.) For the selective creation of a particular quasi-particle state k_s, one wants non-zero coupling constants with $k \to$ condensate and $k' \to k_s$, and also small coupling constants linking the condensate to other quasi-particles. Determining the appropriate SMR field is an iterative process. One can set

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the initial symmetry of $B_{\rm SMR}(\vec{r})$ according to the above discussion, and adjust both $B_{\rm SMR}(\vec{r})$ and $\mathcal{F}(t)$ during the SMR excitation pulse (spatial and spectral chirping) to stay on resonance with the difference in quasi-particle energies and the quasi-particle mode structure (both of which change with depletion of the condensate and accordant reductions in the BH mean field). If the evolution dynamics (i.e. SMR Rabi frequency) is sufficiently slow, then the rotating wave approximation allows us to drop all other states not resonantly coupled[30].

Fig. 3 shows a new calculation of the dependence of SMR coupling constants on condensate atom number in the simple case of a spatially uniform SMR field, again for the MIT sodium condensate in a Cloverleaf trap. The normal coupling constant Ω and the anomalous coupling constant γ are both plotted for two quasi-particle modes that are degenerate at $\tilde{\omega}_k = 26$ when $N = 1$. Note that the coupling to the higher energy mode grows significantly as N is increased; this is consistent with the relative ease with which this shape oscillation has been excited experimentally using a simple trap potential variation[7]. Note also that the coupling to the lower energy mode, with a spatially uniform SMR field, remains very small for all N considered. We are currently investigating the use of SMR fields employing tailored spatial symmetries and chirping techniques to excite specific quasi-particles not well coupled to simple, resonant trap potential modulations (e.g. the lower energy mode shown in Fig. 3).

In this paper, we investigated high energy collective excitations (i.e. quasi-particles) in trapped Bose condensates. These investigations were motivated by recent studies revealing the rich chaotic dynamics involved in such systems. It is interesting to note from our numerical computation that quasi-particle energy levels are basically regular for the MIT trap below $\omega_k = \omega_r = 13(\omega)$, presumably because the radial ($\omega_r = \omega_x = \omega_y$) and axial ($\omega_z$) trap frequencies are significantly different, such that the families of quasi-particles studied here are adiabatically well connected with levels of different radial excitation levels. Interesting level crossing behavior becomes evident when the chemical potential μ becomes of the order of the higher energy shape oscillation mode [i.e. $\omega_k = 2\omega_r = 26(\omega_z = \omega)$]. The detailed crossing/anticrossing character of the quasi-particle level structure will be studied in future work. We also discussed spatial magnetic resonance, or SMR, a technique for the selective creation of quasi-particles and coherent superpositions of quasi-particles. We presented new calculations for the excitation of high energy quasi-particles in the MIT trap using SMR, outlined additional SMR calculations we will pursue in future work, and discussed possible experimental ramifications.

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