Bose-Einstein condensates in spatially periodic potentials

Kirstine Berg-Sørensen[1] and Klaus Mølmer[2]
[1]*Niels Bohr Institute, Ørsted Laboratory, Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark*
[2]*Institute of Physics and Astronomy, University of Aarhus, DK-8000 Århus C, Denmark*
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We investigate theoretically the properties of a Bose-Einstein condensate located in a spatially periodic potential. The excitations of the condensate are obtained from linear equations involving the periodic potential and the periodic condensate density. The Bloch ansatz therefore applies and the excitation spectrum exhibits band structure. If the periodic potential is accelerated, the condensate may undergo Bloch oscillations in the accelerated frame, corresponding to an acceleration without spreading of the entire condensate.
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I. INTRODUCTION

Since the first observation of Bose-Einstein condensation in trapped dilute gases [1–3] the experimental developments in this field have advanced rapidly. Applications of Bose-Einstein condensates have been proposed, and the properties of condensates in different circumstances have become a matter of practical interest. In this work we study the influence of a spatially periodic external potential on the properties of a Bose-Einstein condensate. Such a periodic potential may be induced by a far-off-resonant laser field, and with present trapped condensates it is possible to have a condensate extending over many periods of such a field. The single atom behavior in a periodic potential has been extensively studied in connection with laser cooling and atom optics [4], and, recently, the issue of quantum transport has been addressed both theoretically and experimentally [5]. Our study of condensates in periodic potentials thus both serves to generalize these studies to the case of interacting particles, and it presents a new setting for condensate dynamics where new tools for diagnostics and manipulation of condensates may be suggested. The system of an interacting condensate in a periodic potential complements the situation in optical lattices [6], where interactions can usually be neglected and where dissipation due to spontaneous emission of light plays an important role when the individual atoms localize in different potential minima.

II. THE GROSS-PITAEVSKII EQUATION FOR ATOMS IN A PERIODIC POTENTIAL

We consider a zero-temperature Bose-Einstein condensate of atoms with mass M. The atoms interact by elastic collisions and their low kinetic energies permit a replacement of their short-range interaction by a contact term, so that the single-particle wave function obeys the Gross-Pitaevskii equation,

$$\left[-\frac{\hbar^2}{2M}\nabla^2+V_{\rm ext}(\vec{r})+Ng|\psi(\vec{r})|^2\right]\psi(\vec{r})=\mu\psi(\vec{r}). \quad (1)$$

We consider a condensate extending over many periods of a one-dimensional periodic potential,

$$V_{\rm ext}(x)=V_0\cos\kappa x. \quad (2)$$

All our calculations will be for the corresponding one-dimensional problem [7].

Let N denote the number of atoms per period $2\pi/\kappa$ of the periodic potential. When the Gross-Pitaevskii equation is considered in one dimension, the density of the atoms in the two orthogonal directions must be specified, hereby attributing the coefficient g dimension of energy times length. Very elongated condensates of length ~ 300 μm and with radii of ~ 17 μm have been produced with $\sim 5\times 10^6$ sodium atoms [8]. If we assume that such a condensate is introduced in a potential with a period of roughly 1 μm (half the wavelength of an off-resonant laser beam), we obtain N on the order of 10 000 and g on the order of $0.001(\hbar^2\kappa^2/M)\kappa^{-1}$. We present calculations for this choice of parameters.

A comment on what we mean by the number of atoms N may be in order: The physical situation is that a much larger number of atoms KN are distributed over K periods of the potential. For a weak modulation of the periodic potential, these atoms occupy a common wave function extending over the entire potential. A given period is thus not populated by a definite number of atoms but by a binomial distribution, converging to a Poisson distribution in the limit of large K. When the potential modulation increases, we expect to see the condensate break up into separate condensates, and the lowest energy is obtained with a specific number of atoms in each well, because an imbalance effectively corresponds to an excitation of the system. Although there seems to be a large physical difference between the united and the fragmented condensate, we expect the quantitative signature to be small since the Gross-Pitaevskii equation only differs insignificantly for the two cases: our Eq. (1) is the one that follows from a Poisson distribution ansatz, whereas for a number state ansatz the factor N is replaced by $N-1$. This difference is usually neglected in treatments of Bose condensates. Also for excitations, to be described below, it has been shown that there is little quantitative difference between results obtained with a definite number and with a Poisson distribution, [9], and we therefore believe that our calculations for the condensate density and for the spectrum of excitations of the system are reliable both for small and for large potential modulation.

The condensate ground state is periodic (note that the nonlinear term in the Gross-Pitaevskii equation is perfectly consistent with this property), and the wave function need only be considered on a single period of the potential. A simple and efficient solution of Eq. (1) is obtained by the method of steepest descent, i.e., a propagation in imaginary time τ, replacing $\mu\psi(x)$ by $-(\partial/\partial\tau)\psi(x,\tau)$ on the right-hand side of Eq. (1). In the long-time limit the wave function norm decays with the rate μ, and the renormalized wave function is the desired solution $\psi(x)$.

The results of this numerical treatment may be compared with the ones of the Thomas-Fermi approximation, which neglects the kinetic energy operator in Eq. (1) and yields the expression

$$|\psi^{\mathrm{TF}}(x)|^2=\max\{[\mu-V_{\mathrm{ext}}(x)]/(Ng),0\} \tag{3}$$

for the single particle density. The single-particle energy μ is determined by the normalization of $\psi(x)$ to unity. For $V_0<Ng/(2\pi/\kappa)$ the density is positive everywhere, and μ has the same value as for a homogenous gas, $\mu=Ng/(2\pi/\kappa)$ $(=1.59\hbar^2\kappa^2/M$ for our choice of parameters). For a larger modulation V_0 the atoms fill up the cos potential to a value $\mu<V_0$ and an explicit integration of the distribution establishes the connection between μ and N, g, and V_0: $Ng/(2\pi/\kappa)=\mu-\mu\cos^{-1}(\mu/V_0)/\pi+\sqrt{V_0^2-\mu^2}/\pi$. There is good agreement between the steepest-descent numerical solution of Eq. (1) and the Thomas-Fermi approximation.

III. EXCITATIONS

Excitations out of the condensate may be driven and investigated ''spectroscopically.'' They will be populated if the condensate is at a finite temperature T, and they provide the noncondensed fraction of atoms at zero temperature. The excitations are determined from linear equations, treating the density of the condensed atoms as a fixed background.

The contribution to the Hamiltonian from noncondensed atoms can be written in the canonical form

$$\delta H=\alpha\hat{P}^2/2+\sum_{k\neq 0}\hbar\omega_k g_k^\dagger g_k,\quad [g_k,g_{k'}^\dagger]=\delta_{kk'}, \tag{4}$$

where we have introduced the Bogoliubov transformation of the atomic field operators, $\hat{\Psi}(\vec{r})=\sqrt{N}\psi(\vec{r})+\delta\hat{\Psi}(\vec{r})$ [10],

$$\delta\hat{\Psi}(\vec{r})=\sum_k\,[U_k(\vec{r})\hat{g}_k-V_k^*(\vec{r})\hat{g}_k^\dagger]. \tag{5}$$

The functions $U_k(\vec{r}),V_k(\vec{r})$ fulfill the coupled Bogoliubov–de Gennes equations [10]

$$\begin{aligned}&[L+2gN|\psi(\vec{r})|^2]U_k(\vec{r})-gN|\psi(\vec{r})|^2V_k(\vec{r})=\hbar\omega_k U_k(\vec{r}),\\&[L+2gN|\psi(\vec{r})|^2]V_k(\vec{r})-gN|\psi(\vec{r})|^2U_k(\vec{r})=-\hbar\omega_k V_k(\vec{r}),\end{aligned} \tag{6}$$

where $L=-(\hbar^2/2M)\nabla^2+V_{\mathrm{ext}}(\vec{r})-\mu$, and they are subject to the normalization and orthogonality relations:

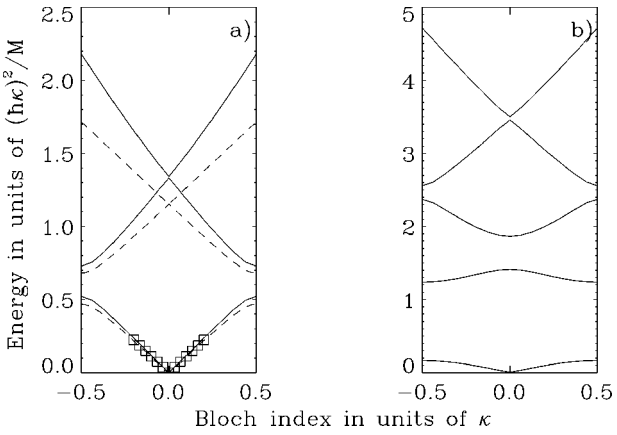

FIG. 1. Excitation spectra as functions of the Bloch index q. In part (a), $V_0=\hbar^2\kappa^2/M$; solid lines: numerical solution of Eq. (6), dashed lines: numerical solution of Eq. (11) and open squares: the analytical expression (12). In part (b), $V_0=3\hbar^2\kappa^2/M$.

$$\int d^3\vec{r}[U_k(\vec{r})U_{k'}^*(\vec{r})-V_k(\vec{r})V_{k'}^*(\vec{r})]=\delta_{kk'}. \tag{7}$$

The excitation of the condensate described by $\alpha\hat{P}^2/2$ in Eq. (4) is the gapless Goldstone mode resulting from the U(1) symmetry breaking [10]. It describes the collapse of the global phase of the condensate, a quantity of relevance for matter wave interference with another condensate. We shall return to a discussion of phase diffusion at the end of our treatment of the excitation spectrum.

The equations (6) are linear and show the usual translation symmetry for periodic problems, which implies that Bloch's theorem applies for the solutions U_k, V_k, i.e., they can be chosen as periodic functions multiplying plane wave factors $\exp(iqx)$. For each value of q in the first Brillouin zone $-\kappa/2<q<\kappa/2$, a discrete set of eigenfunctions are found, and when q is varied these provide the energy bands $E_n(q)=\hbar\omega_n(q)$ for excitations of the system. Examples of the resulting band structure are presented as solid lines in Fig. 1 for the two different values of the potential strength $V_0=\hbar^2\kappa^2/M$ and $3\hbar^2\kappa^2/M$. In Fig. 2 the energy bands are shown as functions of the potential strength.

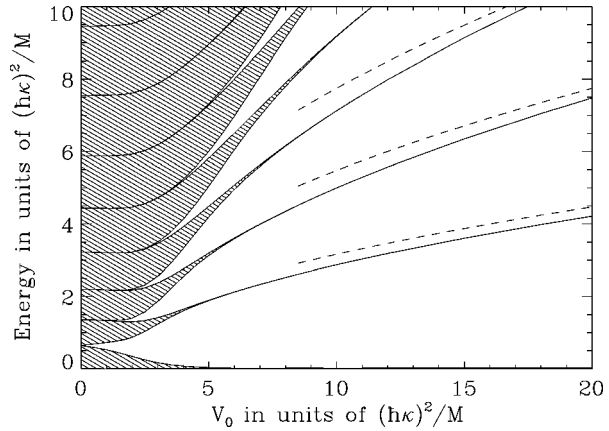

FIG. 2. Energy bands (hatched regions) and band gaps as functions of the potential depth V_0. The dashed lines indicate the discrete eigenvalues for separate condensate fragments.

We may obtain a simpler, approximate equation for the excitations, if we rewrite the Bogoliubov–de Gennes equations,

$$[L+gN|\psi(\vec{r})|^2]\psi_k(\vec{r})=\hbar\omega_k\phi_k(\vec{r}),$$
$$[L+3gN|\psi(\vec{r})|^2]\phi_k(\vec{r})=\hbar\omega_k\psi_k(\vec{r}), \tag{8}$$

where we have introduced $\psi_k(\vec{r})=[U_k(\vec{r})+V_k(\vec{r})]/\sqrt{2}$ and $\phi_k(\vec{r})=[U_k(\vec{r})-V_k(\vec{r})]/\sqrt{2}$. The idea is now to neglect the kinetic energy operator in places where it is relatively least significant. In the operator $[L+3Ng|\psi(\vec{r})|^2]$ the kinetic energy may be neglected in comparison with the remaining term equal to $2[\mu-V_{\rm ext}(\vec{r})]$ in the Thomas-Fermi approximation. Thus, the second equation in Eq. (8) can be formally solved for $\phi_k(\vec{r})$ and upon insertion in the first equation we obtain a single eigenvalue equation,

$$2[\mu-V_{\rm ext}(\vec{r})][L+Ng|\psi(\vec{r})|^2]\psi_k(\vec{r})=(\hbar\omega_k)^2\psi_k(\vec{r}). \tag{9}$$

Subsequently we make the ansatz, $\psi_k(\vec{r})=W_k(\vec{r})\psi(\vec{r})$, and use that $\psi(\vec{r})$ solves the Gross-Pitaevskii equation, to get the equation

$$-\frac{\hbar^2}{M}[\mu-V_{\rm ext}(\vec{r}))[\psi(\vec{r})\nabla^2W_k(\vec{r})+2\nabla\psi(\vec{r})\nabla W_k(\vec{r})]$$
$$=(\hbar\omega_k)^2W_k(\vec{r})\psi(\vec{r}). \tag{10}$$

As the last step, we replace $\psi(\vec{r})$ by $\psi^{\rm TF}(\vec{r})$ and we note that $\nabla\psi^{\rm TF}(\vec{r})/\psi^{\rm TF}(\vec{r})=-\nabla V_{\rm ext}(\vec{r})/\{2[\mu-V_{\rm ext}(\vec{r})]\}$, so that we get the equation

$$-\frac{\hbar^2}{M}[\mu-V_{\rm ext}(\vec{r})]\nabla^2W_k(\vec{r})+\frac{\hbar^2}{M}\nabla V_{\rm ext}(\vec{r})\nabla W_k(\vec{r})$$
$$=(\hbar\omega_k)^2W_k(\vec{r}). \tag{11}$$

Equation (11) generalizes the result of Ref. [13] to arbitrary potentials, and it is in agreement with a hydrodynamical analysis [14].

If we include the periodic potential as a perturbation in Eq. (11), and if we expand $W_k(\vec{r})$ on the functions e^{iqx} and $e^{i(q\pm k)x}$, we obtain an analytical approximation for the lowest band

$$\hbar\omega_q=\sqrt{2\mu\frac{\hbar^2q^2}{2M}\left(1-\frac{V_0^2}{2\mu^2}\right)}, \tag{12}$$

indicated by open squares in Fig. 1(a). The approximation skips a couple of derivatives, and in the homogeneous case where $V_0=0$ it does not provide the second term in the exact expression $\hbar\omega_q=\sqrt{2\mu(\hbar^2q^2/2M)+(\hbar^2q^2/2M)^2}$, readily obtained from Eq. (6). This omission clearly accounts for the discrepancy at high energies between the exact excitation spectrum and the numerical solution to Eq. (11), shown by dashed lines in Fig. 1(a).

By assuming that W_k is a superposition of traveling waves, $\exp(iqx)$ and $\exp[i(q-\kappa)x]$ near the $q=\kappa/2$ zone boundary, we can also determine the energy gap, and for V_0 smaller than μ we get a gap of $\Delta E=V_0\sqrt{(\hbar^2\kappa^2/2M)/(8\mu)}$ between the lowest and the first excited band. When V_0 gets very large we are in the situation of independent condensates with N atoms located in each minimum of the periodic potential. The allowed energy bands then converge to discrete excitations, and assuming a harmonic approximation to the potential, we obtain the excitation energies $\hbar\omega_k=\sqrt{V_0/(\hbar^2\kappa^2/M)}\sqrt{k(k+1)/2}\hbar^2\kappa^2/M$, $k=1,2,\ldots$ [11]. These analytical predictions are in good agreement with the numerical results and are indicated by dashed lines in Fig. 2.

Let us come back to the issue of phase diffusion of the Bose-Einstein condensate. For brevity, we discuss this issue within a symmetry-breaking framework; the same conclusions can be reached with a definite number of particles, where one would discuss the dephasing of an entangled state with different numbers of particles populating different wells [12]. Phase differences between wells represent an excitation of the system, which is already accounted for by the Bogoliubov–de Gennes treatment. This is more easily seen if we rewrite the discrete sum in Eq. (4) in terms of conjugate pairs of ''momenta'' and harmonically bound ''positions'' $(\hat{P}_k,\hat{Q}_k)$. As in a single-particle problem, where the ground state becomes degenerate if the wells decouple completely, a number of the condensate excitation energies converge to zero $(\omega_k\to0)$, and this implies that a number of ''free'' quasiparticles with ''momenta'' $\hat{P}_k$ appear in addition to the one representing the global phase in Eq. (4). In [11], it is explicitly shown for a double-well potential how a single excitation determined by functions $U(x),V(x)$ with opposite signs in the two wells, describes the relative phase of the two condensate components as such a harmonically bound variable. In the limit of separate condensates the excitation energy approaches zero, and the functions $U(x),V(x)$, in fact, yield new values for the quantity α, predicting the correct independent time scales for phases diffusion of the separated condensate components.

In our problem, the lowest energy band, as shown in Fig. 2, is associated with such phase variations across the periodicity of the potential. The Bloch-index q generalizes the odd-even distinction in the double well, and in this context it mimics a Bloch ansatz for the phase variation through the lowest excitation functions $U_q(x),V_q(x)$ obtained for given values of q. In Fig. 2 it is shown that the excitation energies of the lowest band decrease when the potential wells get deeper. Thus, a whole series of Goldstone modes appear, and rather than using the Bloch ansatz, we may form new modes corresponding to phase variables, associated with individual wells. As the calculations in [11] clearly indicate, each fragment acquires a phase diffusion term $\alpha_i\hat{P}_i^2$, with a resulting lifetime of the local phase, comparable to the value obtained within the Thomas-Fermi approximation in a harmonic well with same curvature [11],

$$\tau_c=\hbar\left(\sqrt{\frac{V_0\kappa^2}{3}}\frac{g}{2}\right)^{-2/3}N^{-1/6}. \tag{13}$$

IV. COLLECTIVE CONDENSATE DYNAMICS, BLOCH OSCILLATIONS

We may induce a collective dynamics of the whole condensate by temporally modifying the external potential $V_{\rm ext}$. Experiments have addressed the behavior of condensates in temporally modulated harmonic oscillator traps [15], and damping of condensate oscillations [16] and depletion of the condensate [17] in such situations are topics of current interest.

We consider the case where a constant force field is added along the periodic potential, $V_{\rm ext}(x) \rightarrow V_{\rm ext}(x) - Fx$. A constant external force is equivalent to a constant acceleration of the periodic potential, easily realized experimentally by application of laser fields with constant frequency drifts. In recent experimental works [5,18,19], this situation was studied for the dynamics of independent atoms, and concepts developed in solid state physics were observed: Bloch oscillations, Zener breakdown, Wannier-Stark ladders. In the laboratory frame, the atoms in the lowest band of the band structure are accelerated along with the potential in a dissipation free way, and we shall present the theory for this process applied to a Bose-Einstein condensate.

We wish to solve the time-dependent Gross-Pitaevskii equation

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \left(\frac{p^2}{2M} + V_{\rm ext}(x) + Ng|\psi(x,t)|^2 - Fx \right) \psi(x,t), \tag{14}$$

where $p = -i\hbar \partial/\partial x$. If we make the ansatz, $\psi(x,t) = \exp[iq(t)x]u(x,t)$ and if we set $q(t) = Ft/\hbar$ we obtain the equation for $u(x,t)$:

$$i\hbar \frac{\partial}{\partial t}u(x,t) = \left(\frac{[p+q(t)]^2}{2M} + V_{\rm ext}(x) + Ng|u(x,t)|^2 \right) u(x,t). \tag{15}$$

Within an adiabatic approximation $u(x,t)$ is given by $u_{q(t)}(x)$ multiplied by a phase factor, where $u_q(x)$ solves the eigenvalue equation

$$\left(\frac{(p+q)^2}{2M} + V_{\rm ext}(x) + Ng|u_q(x)|^2 \right) u_q(x) = \mu(q) u_q(x). \tag{16}$$

One might have suggested this equation for the computation of the band structure of the condensate in a periodic potential. Note, however, that it has an entirely different physical meaning, since it determines the time-dependent state of the condensate and the number q is a given function of time. We recall the approximate character of Eq. (16). We are presently studying the solutions of Eq. (15) numerically to verify to which extent the adiabaticity assumption may be applied to our nonlinear problem.

The solution of Eq. (16) can be determined by the steepest-descent method, and if this were an independent particle problem, we would obtain the expectation value of the particle velocity as $v(t) = \hbar^{-1} \partial \mu(q)/\partial q$ evaluated at $q(t)$ [20]. Now, we are dealing with a nonlinear problem, and this expression is not valid. Given the solution of Eq. (16), however, it is no problem to obtain the mean velocity of the atoms by direct computation of the expectation value of the momentum operator. For q values outside the first Brillouin zone, we get a periodic function corresponding to the extended zone scheme representation of the energy spectrum in solid state physics. This is exactly what we want, and it is this periodic behavior of the particle velocity that is referred to as Bloch oscillations. In the case of an accelerated potential, in the laboratory frame the oscillations are superimposed on a steady acceleration at F/M. See Ref. [19] for different physical pictures of this acceleration of independent atoms. We present in Fig. 3 numerical results for $v(q)$ obtained for different values of the potential depth V_0. Recall that q is a function of time, controlled experimentally by the rate of acceleration of the periodic potential. For shallow potential wells, the adiabatic following of the lowest state of the system requires an abrupt change in velocity at each Brillouin zone boundary, and in this case the adiabatic assumption will not be valid.

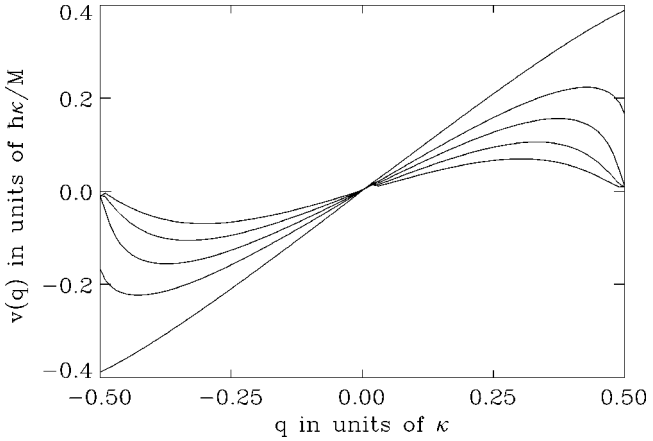

FIG. 3. The mean velocity $v(q)$ for different values of V_0. In an experiment $q = Ft/\hbar$, see text. From above at $q = 0.50$, $V_0/(\hbar^2\kappa^2/M) = 1.,1.5,1.75,2.,2.25$.

V. DISCUSSION

We have investigated the behavior of a Bose-Einstein condensate in a periodic potential. In the static case we have computed the condensate ground state and the band structure of excitations. Numerical results are in good agreement with our simple analytical expressions. It is straightforward to generalize the theory to three-dimensional periodic problems, but in this case it seems worthhwile to apply the effective methods of solid state physics (augmented plane waves, etc.) [20].

We also considered the situation where a constant acceleration is applied to the periodic potential. The prospects to accelerate the atoms without spreading seem attractive for condensates, e.g., in connection with output couplers for atom lasers [21]. If the transverse density of the atoms is not a constant, one has to solve the corresponding 2D or 3D problem, and the dynamics of the condensate may get quite complex. This analysis should be carried out together with a more detailed analysis also of the transient behavior when the atoms are exposed to the periodic potential, and when they eventually leave this potential.

Apart from quantitative differences in excitation spectra

and in the Bloch oscillations of the atoms in an accelerated potential, we imagine that, in particular, breakdown of our simplifying assumptions may cause the most dramatic differences between the behavior of interacting and noninteracting atoms. Transverse instabilities have been mentioned [7], and we recall that for our analysis of Bloch oscillations, the adiabaticity criterion for non-interacting particles of Ref. [19] cannot immediately be applied; we must both consider the passage of the entire condensate to collectively excited states and depletion of the condensate during the acceleration. *A priori*, we imagine that parameters exist so that the adiabaticity assumption is fulfilled, and we may even imagine that the lack of adiabaticity in higher bands causes a Zener breakdown so that noncondensed atoms are not accelerated along with the condensate, hence a filtering process may occur. A temporal variation of the periodic potential, e.g., a harmonic oscillation in time [22], may also address the condensate and the noncondensed cloud in different ways, and could be a way to excite and investigate different ''sounds'' in the system.

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