The effect of a boson condensate on the phonon spectrum

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In this paper the author shows that the presence of a condensate of a nonideal Bose gas interacting with phonons leads to the appearance of an additional phonon mode and to the renormalization of the spectra of the boson and phonon subsystems. Allowing for the nonideality of the Bose gas makes it possible to explain the experimental data on the sound velocity in high-T_c materials.

Experimental data suggests that the sound velocity in high-T_c materials increases as the temperature of the sample decreases.[1] On the other hand, the standard BCS theory predicts "softening" of phonon modes. One of the alternative high-temperature superconductivity theories currently developed is the bipolaron model.[2] A characteristic feature of this model is that polarons in high-T_c materials couple into bipolarons (a bipolaron is a bound state of two polarons), which at low concentrations are bosons. Superconductivity in this model appears when a Bose condensate of bipolarons emerges.

The present article attempts to explain the experimental data on the sound velocity from the standpoint of the bipolaron model. For an ideal boson gas this problem was solved in Ref. 3. Here it is assumed that the phonons in a crystal interact with the nonideal boson gas of bipolarons. Such a system is described by the following Hamiltonian:

$$H=\sum_p\left[\left(\frac{p^2}{2m}-\mu\right)b_p{}^+b_p+\omega_p d_p{}^+d_p\right]+\sum_{p,q}\left(\frac{\varkappa_q}{V^{1/2}}b^+_{p+q}b_pd_q+\text{H.c.}\right)+\sum_{\substack{p_1+p_2=\\=p_1'+p_2'}}\frac{\nu(p_1-p_1')}{2V}b_{p_1}{}^+b_{p_2}{}^+b_{p_2'}b_{p_1'}, \qquad (1)$$

where b_p and b_p^+ are the operators of annihilation and creation of bosons with momentum p, d_p and d_p^+ are similar operators for phonons, $\varkappa_q$ is the boson-phonon coupling constant, V and μ the volume and chemical potential of the system, ω_p the phonon frequency, m the boson mass (the bipolaron mass). At a temperature T lower than the critical temperature there appears a Bose condensate, which can be isolated by setting $b_0=b_0^+=[N_0(T)]^{1/2}$, with $N_0(T)$ the number of bosons in the condensate. As a result the Hamiltonian assumes the form

$$H_2=\sum_{p\neq0}\Big[\varepsilon_pb_p{}^+b_p+\omega_pd_p{}^+d_p+(\varkappa_pn_0{}^{1/2}d_p+\varkappa_p{}^*n_0{}^{1/2}d_{-p}{}^+)(b_p{}^++b_{-p})+\frac{1}{2}\mu_p(b_p{}^+b_{-p}{}^++b_{-p}b_p)\Big]+H_1, \qquad (2)$$

$$H_1=\sum_{p,q\neq0}n_0{}^{1/2}\varkappa_qb^+_{p+q}b_pd_q+\text{H.c.},$$

with $n_0=N_0(T)/V$ the condensate density, $\mu_p=n_0\nu(p)$, and $\varepsilon_p=p^2/2m+\mu_p$. Boson interactions are not considered in what follows and, therefore, the respective term is dropped.

The presence of a condensate leads to mixing of boson and phonon operators in the third term within the square brackets in Eq. (2). Reduction of the quadratic form H_2 to diagonal form requires introducing new operators b' and d' that are linear combinations of the old operators:

$$\begin{pmatrix}b'^+\\b'\\d'^+\\d'\end{pmatrix}=C\begin{pmatrix}b^+\\b\\d^+\\d\end{pmatrix}. \qquad (3)$$

Although the explicit form of matrix C can be obtained in the diagonalization process, it will be of no use to us here. One can easily show that, say, operator b' differs from operator b by a quantity proportional to $\varkappa_p$. When calculating correction terms proportional to $H_1^2\propto\varkappa^2$, allowing for the difference between b' and b in the interaction Hamiltonian leads to excessive accuracy.

Thus, as a result of diagonalization we obtain the Hamiltonian that describes the new excitations,

$$H=\sum_{p\neq0}[E_1(p)b_p{}'^+b_p{}'+E_2(p)d_p{}'^+d_p{}']+H_1,$$
$$H_1=\sum_{p,q\neq0}[n_0(T)]^{1/2}\varkappa_pb'^+_{p+q}b_q{}'d_p{}'+\text{H.c.}+O(\varkappa_p{}^2), \qquad (4)$$

with the spectrum

$$E(p)^2_{1,2}=0.5\{\omega_p{}^2+\varepsilon_p{}^2-\mu_p{}^2\mp[(\omega_p{}^2-\varepsilon_p{}^2+\mu_p{}^2)^2+8|\varkappa_p|^2\times\omega_pn_0(T)p^2/m]^{1/2}\}. \qquad (5)$$

Equation (5) implies that the above reasoning is valid for $\omega_p(\varepsilon_p+\mu_p)\geqslant4n_0^2|\varkappa_p|^2$, since, otherwise, imaginary frequencies appear and the system becomes unstable. This condition does not generally mean that the coupling constant $\varkappa_p$ is small and, hence, according to Eq. (5), the Bogolyubov spectrum of the interacting bosons and the phonon spectrum may undergo a strong modification.

The interaction with the boson condensate also leads to mixing of the phonon and boson variables, which means that both types of excitation are related to lattice-deformation transfer. Hence, at temperatures below the critical there appears an additional acoustic mode.

Note that polariton theory also encounters the problem of diagonalizing a similar quadratic Hamiltonian: diagonalization leads to the appearance of two new branches of elementary excitations with a spectrum similar to (5). The

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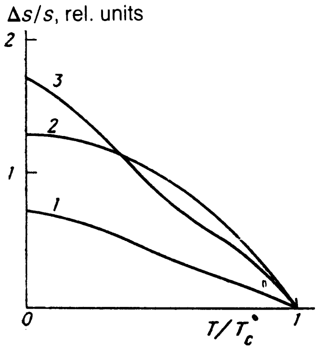

FIG. 1. The temperature dependence of the sound velocity calculated via Eq. (8) for different values of the parameters $\eta_s = ms^2/T_c$ and $\eta_u = n_0(0)v(0)/T_c$: curve 1, $\eta_s = 1$ and $\eta_u = 0.1$; curve 2, $\eta_s = 0.5$ and $\eta_u = 0$ (an ideal Bose gas); and curve 3, $\eta_s = 0.5$ and $\eta_u = 0.1$.

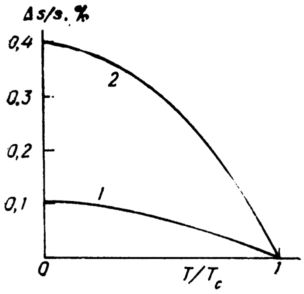

FIG. 2. The experimental data on the temperature dependence of the sound velocity in Y–Ba–Cu–O: curve 1, the data of Ref. 1; curve 2, the data of Bhattacharya *et al.*

main difference is that in our case the mixing of the initial variables occurs only in the presence of a boson condensate.

Equation (5) suggests that the corrections to the energy at small values of the coupling constant $\varkappa$ are proportional to $\varkappa^2$ and, hence, second-order quantum corrections in $\varkappa$ must also be taken into account. Let us do this for the phonon spectrum, since we are interested in the sound velocity. For the sake of simplicity we will call the excitations with a spectrum $E_p = E_1(p)$ bosons and those with the spectrum $\Omega_p = E_2(p)$ phonons. Then the correction to the phonon energy in second-order perturbation theory is

$$\Delta\Omega_p = \left\langle\!\!\left\langle \sum_m \frac{|\langle p,\alpha|H_1|m\rangle|^2}{\Omega_p+\varepsilon_\alpha-\varepsilon_m} \right\rangle\!\!\right\rangle, \tag{6}$$

where $|p,\alpha\rangle$ is the initial state containing a single phonon with momentum p and energy Ω_p and a system of bosons whose state is characterized by variable α and energy ε_α, and $|m\rangle$ an intermediate state with energy ε_m. The angle brackets $\langle\langle ... \rangle\rangle$ stand for the ordinary averaging over the statistical ensemble of bosons. Standard calculations lead to an expression similar to the one obtained in the random-phase approximation:

$$\Delta\Omega_p = -|\varkappa_p|^2 \sum_{k\neq 0} \frac{f_{p+k}-f_k}{\Omega_p+E_k-E_{p+k}} \tag{7}$$

with $f_k = \langle\langle a_k^+ a_k \rangle\rangle = [\exp(-E_k/T) - 1]^{-1}$. As a result, allowing for the correction to the phonon spectrum (5) necessited by the interaction with the condensate at small values of $\varkappa$, one can easily find that

$$\Delta\omega(p) = |\varkappa_p|^2 \left\{ \frac{n_0(T)p^2}{(\omega_p^2+\mu_p^2-\varepsilon_p^2)m} - \sum_{k\neq 0} \frac{f_{p+k}-f_k}{\omega_p+\varepsilon_k-\varepsilon_{p+k}} \right\}. \tag{8}$$

The first term in Eq. (8) is proportional to the condensate density $n_0(T)$, which explains the reduction in the sound velocity $s = \partial\omega(p)/\partial p$ as the temperature grows. To estimate this contribution, we ignore the nonideality of the Bose gas, which leads to the following expression for the correction to the sound velocity:

$$\frac{\Delta s}{s} = \frac{n_0(T)}{ms^3}\chi, \quad \chi = \frac{|\varkappa|^2}{p}.$$

Since $n_0(T)$ is proportional to $1 - (T/T_c)^{3/2}$, it becomes obvious that the sound velocity increase in cooling is related to the increase in the condensate's density. The second term within the braces in (8) also contributes to the correction to the sound velocity, and this contribution may become primary at $T \sim T_c$. The results of numerical calculations are depicted in Fig. 1, and Fig. 2 presents the characteristic experimental curves taken from Refs. 1. Comparison shows that the experimental data on the sound velocity in high-T_c materials can be explained on the basis of the local-pair theory.

Thus, exact allowance for the interaction of phonons with a boson condensate leads to a modification of both the phonon spectrum and the boson spectrum and to observable effects of the type of increase in the sound velocity in cooling and the appearance of an additional acoustic mode.

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