Upper critical field of bipolaron superconductors

A.S. Aleksandrov and D.A. Samarchenko

Moscow Institute of Engineering Physics (Submitted 10 July 1990) Zh. Eksp. Teor. Fiz. **99**, 574–588 (February 1991)

In narrow-band crystals with strong electron-phonon interactions, electrons form bound pairs that are localized at lattice sites, i.e., small-radius bipolarons. We show that for arbitrary concentrations of these pairs the properties of these systems can be described using an equivalent Bose Hamiltonian. For arbitrary bipolaron concentrations we find the upper critical magnetic field $H_{c2}(T)$, including anisotropy. Our predictions of the temperature dependence of the field H_{c2} explain the unusual behavior of this field in the high-temperature superconductors.

INTRODUCTION

The discovery of the high-temperature superconductors by Müller and Bednorz¹ and by Chu and his collaborators² has given a powerful impetus to the development of an ever-increasing number of theories for high-temperature superconductivity.

References 3 and 4 contain discussions of a large amount of experimental data which appear to confirm that superconductivity in the compounds Bi-Sr-Ca-Cu-O, K-Ba-Bi-O, Y(RE)-Ba-Cu-O, and other metallic oxides, is well described by multipolaron strong-coupling theories.^{5,6}

When the condition for formation of small-radius polarons is fulfilled,

$$\lambda \sim f(z) g^2 \omega / D > 1, \tag{1}$$

(here λ is the electron-phonon coupling constant, z the coordination number of the lattice, ω the characteristic phonon frequency, and g^2 the Froehlich interaction constant), a substantial reconstruction of the electronic spectrum takes place, a notable feature of which is the exponential contraction of an original electron band of width 2D into an extremely narrow polaron band.

As the quantity g increases, the effective attraction between carriers due to the static deformation of the lattice also increases; for two electrons on the same site, the magnitude of this shift is $g^2\omega$, i.e., the polaron shift. This attraction is strong enough to balance the Coulomb repulsion, and leads to the formation of bound pairs localized either on a single lattice site (single-site bipolarons) or on two such sites (double-site bipolarons).^{5,6} In Refs. 5 and 6 it was shown that small bipolarons are transported throughout the crystal, forming narrow bipolaron bands. In this case the band motion takes place by way of transitions to virtual depairing states, and the interaction, along with the usual Coulomb and phonon-exchange interactions, includes the exchange of virtual polarons as well.

Taking into account the polaron effect qualitatively changes the nature of the superconducting state: in the intermediate region $\lambda \approx 1$, the normal BCS type of superconductivity is replaced by polaronic superconductivity,⁴ and in the strong-coupling limit $\lambda \gg 1$ it is replaced by bipolaron superconductivity.⁵ In Ref. 7 it was shown that the behavior of the electron-phonon system with strong interactions is identical to the behavior of a charged interacting Bose gas for arbitrary boson concentrations. Along with the earlier Ref. 5, this paper also contains an investigation of the critical magnetic field of a condensate of charged bosons interacting either among themselves⁷ or with lattice impurities.⁵ However, all these calculations were carried out in the limit of low bipolaron concentrations, so that the bipolaron commutation relations were almost Bose-like.

In this paper we will describe a method that can be used to determine the temperature dependence of the upper critical field H_{c2} for the spatially homogeneous state of the bipolaron system.⁵ This state is obtained either in the case of a weak dynamic interaction $v \leqslant t$ for arbitrary concentrations n_b of bipolarons or in general for low bipolaron concentrations $n_b \leqslant t/v$ (where t is the bipolaron overlap integral). It is found that H_{c2} differs from zero even in the absence of dynamic interactions between the particles, due to kinematic interactions that emerge as a consequence of the bipolaron commutation relations.

1. GREEN'S FUNCTION FOR SMALL BIPOLARONS IN A QUANTIZING MAGNETIC FIELD

The representation obtained in Ref. 7 for the bipolaron Hamiltonian in terms of Bose operators cannot be used as the basis for a diagram technique that is convenient for calculating the properties of this system. Hence we will use the diagram technique developed in the preprint Ref. 8 for ferromagnetic systems.

Let us rewrite the bipolaron Hamiltonian in terms of the pseudospin formalism:⁵

$$\mathcal{H} = \mu \sum_{\mathbf{m}} S_{\mathbf{m}}^{z} - \sum_{\mathbf{m}, \mathbf{m}' \neq \mathbf{m}} t(\mathbf{m} - \mathbf{m}') S_{\mathbf{m}}^{+} S_{\mathbf{m}'}^{-} + \sum_{\mathbf{m}, \mathbf{m}' \neq \mathbf{m}} v(\mathbf{m} - \mathbf{m}') S_{\mathbf{m}}^{z} S_{\mathbf{m}'}^{z}, \qquad (2)$$

where

 $S_{m^{z}} = i/_{2} - b_{m} + b_{m}, \quad S_{m} + = b_{m} +, \quad S_{m} - = b_{m},$

here μ is the chemical potential, $t(\mathbf{m} - \mathbf{m}')$ is the bipolaron overlap integral, $v(\mathbf{m} - \mathbf{m}')$ is the effective bipolaron interaction, $b_{\mathbf{m}}^{+}$ and $b_{\mathbf{m}}$ are creation and annihilation operators for bipolarons, and **m** labels the lattice sites.

In order to formulate the rules of the diagram technique, let us write another Hamiltonian:

$$\tilde{\mathcal{H}} = \mu \sum_{\mathbf{m}} \tilde{S}_{\mathbf{m}}^{z} - \sum_{\mathbf{m}, \mathbf{m'} \neq \mathbf{m}} t(\mathbf{m} - \mathbf{m'}) \tilde{S}_{\mathbf{m}}^{+} \tilde{S}_{\mathbf{m'}}^{-} + \sum_{\mathbf{m}, \mathbf{m'} \neq \mathbf{m}} \tilde{S}_{\mathbf{m}}^{z} \tilde{S}_{\mathbf{m'}}^{z} v(\mathbf{m} - \mathbf{m'}), \qquad (3)$$

where

$$\widetilde{S}_{\mathbf{m}}^{z} = \frac{1}{2} - a_{\mathbf{m}}^{+} a_{\mathbf{m}} - 2f_{\mathbf{m}}^{+} f_{\mathbf{m}}, \qquad (4)$$

$$\widetilde{S}_{\mathbf{m}}^{+} = a_{\mathbf{m}}^{+} - a_{\mathbf{m}}^{+} a_{\mathbf{m}}^{+} a_{\mathbf{m}}^{-} - 4a_{\mathbf{m}}^{+} f_{\mathbf{m}}^{+} f_{\mathbf{m}}, \quad \widetilde{S}_{\mathbf{m}}^{-} = a_{\mathbf{m}},$$

and a_m^+ and a_m are the usual Bose creation and annihilation operators, while f_m^+ and f_m are Fermi creation and annihilation operators. By direct verification we can show that the operators \tilde{S}_m^{\pm} satisfy the same commutation rules as $S_m^{z\pm}$.

The space in which the new operators act is infinitedimensional, in contrast to the initial space (which is finitedimensional because only one bipolaron can sit on a given lattice site). Using the commutation properties of $S_m^{z\pm}$ we can show that the average of a product of spin operators $S_m^{z\pm}$ calculated over the physical space can be expressed in terms of an average of $\tilde{S}_m^{z\pm}$ using the following relation:

$$\langle \dots S_{\mathbf{m}}^{+} \dots S_{\mathbf{m}'}^{-} \dots S_{\mathbf{m}''}^{z} \dots \rangle = \langle \hat{P} \dots \tilde{S}_{\mathbf{m}}^{+} \dots \tilde{S}_{\mathbf{m}'}^{-} \dots \tilde{S}_{\mathbf{m}''}^{z} \dots \rangle, \qquad (5)$$

where $\hat{P} = \exp(i\pi\Sigma_{\rm m}f_{\rm m}^+f_{\rm m})$ is a projection operator onto the physical space and $\langle ... \rangle = \operatorname{Sp}\{...\exp(-\beta\mathcal{H})\}/$ $\operatorname{Sp}\{\exp(-\beta\mathcal{H})\}$, with $\beta = 1/T$ (here and in what follows we set $k_B = \hbar = c = 1$).

Let us introduce the Bose Green's function:

$$G_{\mathbf{m}\mathbf{m}'}(\tau_{1}-\tau_{2}) = -\langle \hat{P}T_{\tau}a_{\mathbf{m}}(\tau_{1})a_{\mathbf{m}'}^{\dagger}(\tau_{2})\rangle$$

$$= \begin{cases} \langle \hat{P}a_{\mathbf{m}}(\tau_{1})a_{\mathbf{m}'}^{\dagger}(\tau_{2})\rangle, \ \tau_{1} > \tau_{2}, \\ \langle \hat{P}a_{\mathbf{m}'}^{\dagger}(\tau_{2})a_{\mathbf{m}}(\tau_{1})\rangle, \ \tau_{1} < \tau_{2}, \end{cases}$$

$$(6)$$

where τ is the "imaginary" time, and the Fermi Green's function

$$F_{\mathbf{m}\mathbf{m}'}(\tau_1 - \tau_2) = -\langle \hat{P}T_{\tau}f_{\mathbf{m}}(\tau_1)f_{\mathbf{m}'}^+(\tau_2)\rangle.$$
(7)

We note a number of properties of the function F_{mm} , (τ) : the presence of the projection operator \hat{P} implies that

$$F_{\mathbf{m}\mathbf{m}'}(\tau < 0) = F_{\mathbf{m}\mathbf{m}'}(\tau + \beta), \tag{8}$$

$$F_{\mathbf{m}\mathbf{m}'}(\tau) = \sum_{j} F_{\mathbf{m}\mathbf{m}'}(\omega_{j}) e^{-i\omega_{j}\tau}, \quad \omega_{j} = 2\pi j T, \quad j = 0, \pm 1, \pm 2, \dots,$$

i.e., the expansion of the function F in terms of the Matsubara frequencies is the same as the one for the Bose Green's function. Since only the product⁸ $f_m^+ f_m$ enters into the definition (3), we find that

$$F_{\mathbf{m}\mathbf{m}'}(\tau) = \delta_{\mathbf{m}\mathbf{m}'} F(\tau). \tag{9}$$

From this we see that the initial system of bipolarons described by the Hamiltonian (2) is equivalent to a system of two interacting Bose and Fermi fields a_m and f_m , with the unique features mentioned above. In the representation (4) the Hamiltonian (3) will appear as follows:

$$\tilde{\mathscr{H}} = -\mu \sum_{\mathbf{m}} a_{\mathbf{m}}^{+} a_{\mathbf{m}}^{-} 2\mu \sum_{\mathbf{m}} f_{\mathbf{m}}^{+} f_{\mathbf{m}}^{-} \sum_{\mathbf{m}, \mathbf{m}' \neq \mathbf{m}} t(\mathbf{m} - \mathbf{m}') a_{\mathbf{m}}^{+} a_{\mathbf{m}'}^{-} + \sum_{\mathbf{m}, \mathbf{m}' \neq \mathbf{m}} t(\mathbf{m} - \mathbf{m}') a_{\mathbf{m}}^{+} a_{\mathbf{m}}^{+} a_{\mathbf{m}}^{-} a_{\mathbf{m}'}^{+} + 4 \sum_{\mathbf{m}, \mathbf{m}' \neq \mathbf{m}} t(\mathbf{m} - \mathbf{m}') a_{\mathbf{m}}^{+} f_{\mathbf{m}}^{+} f_{\mathbf{m}}^{-} a_{\mathbf{m}'}^{-} + \sum_{\mathbf{m}, \mathbf{m}' \neq \mathbf{m}} v(\mathbf{m} - \mathbf{m}') [a_{\mathbf{m}}^{+} a_{\mathbf{m}} a_{\mathbf{m}'}^{+} + a_{\mathbf{m}'}^{+} + 2a_{\mathbf{m}}^{+} a_{\mathbf{m}} f_{\mathbf{m}'}^{+} f_{\mathbf{m}'}^{-} + 2f_{\mathbf{m}}^{+} f_{\mathbf{m}} a_{\mathbf{m}'}^{+} a_{\mathbf{m}'}^{-} + 4f_{\mathbf{m}}^{+} f_{\mathbf{m}} f_{\mathbf{m}'}^{+} f_{\mathbf{m}'}^{-}].$$
(10)

In a weak magnetic field ($eHa^2 \ll 1$, where *a* is the lattice parameter) the overlap integral of the bipolarons can be written in the following form:⁷

$$t(\mathbf{m}, \mathbf{m}') = t(\mathbf{m} - \mathbf{m}') \exp \left[2ie\mathbf{A}(\mathbf{m}) (\mathbf{m} - \mathbf{m}')\right], \quad (11)$$

where A(m) is the vector potential.

Let us convert the lattice-site representation of the operators (4) to a coordinate representation

$$\psi(\mathbf{r}) = \left(\frac{v_c}{N}\right)^{\frac{1}{2}} \sum_{\mathbf{m}} \delta(\mathbf{r} - \mathbf{m}) a_{\mathbf{m}},$$

$$a_{\mathbf{m}} = \left(\frac{v_c}{N}\right)^{\frac{1}{2}} \int \psi(\mathbf{r}) \delta(\mathbf{r} - \mathbf{m}) d\mathbf{r},$$

$$\varphi(\mathbf{r}) = \left(\frac{v_c}{N}\right)^{\frac{1}{2}} \sum_{\mathbf{m}} \delta(\mathbf{r} - \mathbf{m}) f_{\mathbf{m}},$$

$$f_{\mathbf{m}} = \left(\frac{v_c}{N}\right)^{\frac{1}{2}} \int \varphi(\mathbf{r}) \delta(\mathbf{r} - \mathbf{m}) d\mathbf{r},$$
(12)

where v_C is the volume of a unit cell and N the number of these cells. The Hamiltonian \mathcal{H} can be rewritten in the new representation as follows:

$$\begin{aligned} \widetilde{\mathscr{H}} &= -\mu \int d\mathbf{r} \, \psi^{+}(\mathbf{r}) \, \psi(\mathbf{r}) - 2\mu \int d\mathbf{r} \, \varphi^{+}(\mathbf{r}) \, \varphi(\mathbf{r}) - \int d\mathbf{r} \, d\mathbf{r}' t(\mathbf{r}, \mathbf{r}') \\ &\times \psi^{+}(\mathbf{r}) \, \psi(\mathbf{r}') + \frac{v_{C}}{N} \int d\mathbf{r} \, d\mathbf{r}' \psi^{+}(\mathbf{r}) \, \psi^{+}(\mathbf{r}) \, \psi(\mathbf{r}) t(\mathbf{r}, \mathbf{r}') \, \psi(\mathbf{r}') \\ &+ \frac{v_{C}}{N} \int d\mathbf{r} \, d\mathbf{r}' \psi^{+}(\mathbf{r}) \varphi^{+}(\mathbf{r}) \varphi(\mathbf{r}) t(\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}') \\ &+ \frac{v_{C}}{N} \int d\mathbf{r} \, d\mathbf{r}' v(\mathbf{r} - \mathbf{r}') \left\{ \psi^{+}(\mathbf{r}) \psi(\mathbf{r}) \psi^{+}(\mathbf{r}') \psi(\mathbf{r}') \\ &+ 4\psi^{+}(\mathbf{r}) \psi(\mathbf{r}) \varphi^{+}(\mathbf{r}') \varphi(\mathbf{r}') + 4\varphi^{+}(\mathbf{r}) \varphi(\mathbf{r}) \varphi^{+}(\mathbf{r}') \varphi(\mathbf{r}') \right\}. \end{aligned}$$

In deriving this we have used the fact that

$$t(\mathbf{r}, \mathbf{r}') = \frac{v_C}{N} \sum_{\mathbf{m}, \mathbf{m}' \neq \mathbf{m}} t(\mathbf{m} - \mathbf{m}') \exp[2ie\mathbf{A}(\mathbf{m}) (\mathbf{m} - \mathbf{m}')]$$
$$\times \delta(\mathbf{r} - \mathbf{m}) \delta(\mathbf{r}' - \mathbf{m}'),$$
$$v(\mathbf{r} - \mathbf{r}') = \frac{v_C}{N} \sum_{\mathbf{m}, \mathbf{m}' \neq \mathbf{m}} v(\mathbf{m} - \mathbf{m}') \delta(\mathbf{r} - \mathbf{m}) \delta(\mathbf{r}' - \mathbf{m}').$$

The fundamental thermodynamic properties of this system are determined by correlations over distances $|\mathbf{r} - \mathbf{r}'|$ that are larger than the lattice constant. In this case we can write $t(\mathbf{r}, \mathbf{r}')$ in the following form:

$$t(\mathbf{r}, \mathbf{r}') \approx \delta(\mathbf{r} - \mathbf{r}') t(-i\nabla - 2e\mathbf{A}(\mathbf{r})).$$
(14)

Near the band edge we obtain from expression (14)

$$t(\mathbf{r},\mathbf{r}') \approx \delta(\mathbf{r}-\mathbf{r}') \left\{ t_0 - \frac{[\nabla - 2ei\mathbf{A}(\mathbf{r})]^2}{2m^{**}} \right\}, \qquad (14')$$

where $t_0 = 6t$ (for the case of a simple cubic lattice), and $m^{**} = 1/2ta^2$ is the bipolaron effective mass. Assuming that the Coulomb repulsion is screened over distances $r \sim a$, the effective interaction $v(\mathbf{r} - \mathbf{r}')$ can be treated as short-range.

For specific calculations we will turn to a new representation:

$$\psi(\mathbf{r}) = \sum_{\mathbf{v}} a_{\mathbf{v}} \chi_{\mathbf{v}}(\mathbf{r}), \quad \varphi(\mathbf{r}) = \sum_{\mathbf{v}} f_{\mathbf{v}} \chi_{\mathbf{v}}(\mathbf{r}),$$

where the χ_{ν} are eigenfunctions of the Schrödinger equation in a uniform magnetic field $[\mathbf{A} = (-Hy, 0, 0)]$:

$$\chi_{\mathbf{v}}(\mathbf{r}) = \frac{\exp[i(p_{\mathbf{x}}\mathbf{x}+p_{\mathbf{z}}\mathbf{z})]}{(\pi l^{2})^{\frac{1}{2}}(2^{n}n!)^{\frac{1}{2}}} \exp\left[\frac{(y+p_{\mathbf{z}}l^{2})^{2}}{2l^{2}}\right] H_{n}\left(\frac{y+p_{\mathbf{z}}l^{2}}{l}\right),$$
$$E_{\mathbf{v}} = \left(n+\frac{1}{2}\right)\frac{2eH}{m^{**}} + \frac{p_{\mathbf{z}}^{2}}{2m^{**}},$$
(15)

here $l^2 = (2eH)^{-1}$, $v = (p_x, p_z, n)$; p_x and p_z are the bipolaron momenta, *n* labels the Landau levels, and $H_n(x)$ is a Hermite polynomial. The wave function is normalized to unity.

Although the bipolaron is located in a crystal and, consequently, momentum is not a good quantum number, we need not consider umklapp processes if we limit our calculations to one reciprocal lattice cell, i.e., impose the condition

 $p_x, p_z \ll a_{x,z}$.

Then the Hamiltonian can be rewritten in the following form:

$$\widetilde{\mathscr{H}} = -\mu \sum_{\mathbf{v}} a_{\mathbf{v}}^{+} a_{\mathbf{v}} - 2\mu \sum_{\mathbf{v}} f_{\mathbf{v}}^{+} f_{\mathbf{v}} - \sum_{\mathbf{v}} t_{\mathbf{v}} a_{\mathbf{v}}^{+} a_{\mathbf{v}} + v_{C} \sum_{\mathbf{v}_{\mathbf{v}_{i}} \mathbf{v}_{\mathbf{v}_{i}}} (t_{\mathbf{v}} + v_{0}) Y_{\mathbf{v}_{\mathbf{v}_{v}} \mathbf{v}_{a}}^{\mathbf{v} \mathbf{v}_{i}} a_{\mathbf{v}_{i}}^{+} a_{\mathbf{v}_{a}} a_{\mathbf{v}_{a}} + 4v_{\pi} \sum_{\mathbf{v}_{\mathbf{v}_{i}} \mathbf{v}_{\mathbf{v}_{i}}} (t_{\mathbf{v}} + v_{0}) Y_{\mathbf{v}_{\mathbf{v}} \mathbf{v}_{a}}^{\mathbf{v} \mathbf{v}_{i}} d_{\mathbf{v}}^{+} f_{\mathbf{v}_{i}}^{+} f_{\mathbf{v}_{a}} a_{\mathbf{v}_{a}} + 4v_{C} \sum_{\mathbf{v}_{\mathbf{v}_{i}} \mathbf{v}_{\mathbf{v}_{i}}} v_{0} Y_{\mathbf{v}_{\mathbf{v}} \mathbf{v}_{i}}^{\mathbf{v} \mathbf{v}_{i}} f_{\mathbf{v}_{i}}^{+} f_{\mathbf{v}_{a}}^{+} f_{\mathbf{v}_{a}}^{+} f_{\mathbf{v}_{a}}^{+} d_{\mathbf{v}_{a}}, \qquad (16)$$

where

$$Y_{\nu_2\nu_3}^{\nu\nu_1} = \int d\mathbf{r} \chi_{\nu}^{\cdot}(\mathbf{r}) \chi_{\nu_1}^{\cdot}(\mathbf{r}) \chi_{\nu_2}(\mathbf{r}) \chi_{\nu_3}(\mathbf{r}).$$

Because of what was said above the Hamiltonian (16) does not contain umklapp processes. Since the overlap integral was chosen in the form (14), in the representation (15) it becomes

$$t(-i\nabla - 2e\mathbf{A}(\mathbf{r}))\chi_{\nu}(\mathbf{r}) = t_{\nu}\chi_{\nu}(\mathbf{r}).$$

Let us introduce $\varepsilon_v = -\mu - t_v$, once more rewriting the Hamiltonian:

$$\tilde{\mathscr{H}} = \sum_{\mathbf{v}} \varepsilon_{\mathbf{v}} a_{\mathbf{v}}^{+} a_{\mathbf{v}} - 2\mu \sum_{\mathbf{v}} f_{\mathbf{v}}^{+} f_{\mathbf{v}} + \mathscr{H}_{int}(a_{\mathbf{v}}, f_{\mathbf{v}}),$$

and choose the unperturbed temperature Green's functions in the following way:

$$G_{\mathbf{v}}^{0}(\omega_{j}) = \frac{1}{i\omega_{j} - \varepsilon_{\mathbf{v}}}, \quad F^{0}(\omega_{j}) = \frac{1}{i\omega_{j} - 2\mu}.$$
(17)

We formulate some general rules for the diagram tech nique. The elementary vertices are shown in Fig. 1, while Fig. 2 illustrates a few of the diagrams up to second order for $G_v(\omega_j)$; the wavy line denotes the kinematic interaction $t_v + v_0$. In Fig. 2 we do not include diagrams that lead only to a change in the chemical potential. The function $F_v(\omega_j)$ contains diagrams of the type shown in Fig. 3. Perturbation theory, together with Eq. (9), shows that $F_v(\omega_j) = F(\omega_j)$ holds to all orders. Therefore we can write $F(\omega_j)$ in the following form:

$$F(\omega_j) = \frac{1}{(i\omega_j - X)}, \qquad (18)$$

where X is the self-energy part for the Fermi field, while the fermion density is

$$n_r = (e^{x/r} - 1)^{-1}.$$
 (19)

The vertex factor $Y_{\nu_2\nu_3}^{\nu\nu_1}$ is easy to calculate; however, in the discussion that follows we will consider only interactions between particles in the lowest Landau level, in which case $Y_{\nu_2\nu_3}^{\nu\nu_1}$ becomes

$$Y_{p_{23}p_{23}, p_{23}p_{23}, p_{23}p_{23}}^{p_{2}p_{23}, p_{23}p_{23}} = \frac{1}{l(2\pi)^{1/s}} \, \delta_{p_{x}+p_{x1}, p_{x3}+p_{x3}} \\ \times \, \delta_{p_{z}+p_{21}, p_{23}+p_{23}} \exp\left[-\frac{l^{2}}{2} \sum_{i}^{4} p_{x_{i}}^{2} + \frac{l^{2}}{8} \left(\sum_{i}^{4} p_{x_{i}}\right)^{2}\right], \quad (20)$$

where δ_{k_r,k_r} is the Kronecker symbol.

Now consider the bipolaron Green's function, which is defined as follows:

$$G_{\mathbf{m}\mathbf{m}'}^{b}(\tau_{1}-\tau_{2}) = \langle T_{\tau}b_{\mathbf{m}}(\tau_{1})b_{\mathbf{m}'}^{+}(\tau_{2})\rangle = \langle T_{\tau}S_{\mathbf{m}}^{-}(\tau_{1})S_{\mathbf{m}'}^{+}(\tau_{2})\rangle = \langle T_{\tau}S_{\mathbf{m}}^{-}(\tau_{1})S_{\mathbf{m}'}^{+}(\tau_{2})\rangle.$$
(21)

If we substitute the representation (13) for the spin operators in terms of Bose and Fermi operators into (21), we obtain

$$G_{\mathbf{m}\mathbf{m}'}^{b}(\tau) = G_{\mathbf{m}\mathbf{m}'}(\tau) + G_{\mathbf{m}\mathbf{m}'}^{\mathrm{II}}(\tau) + F_{\mathbf{m}\mathbf{m}'}^{\mathrm{II}}(\tau), \qquad (22)$$

where

$$G_{\mathbf{m}\mathbf{m}'}^{11}(\tau) = -\langle \hat{P}T_{\tau}a_{\mathbf{m}}(0)a_{\mathbf{m}'}^{+}(\tau)a_{\mathbf{m}'}^{+}(\tau)a_{\mathbf{m}'}(\tau)\rangle,$$

$$F_{\mathbf{m}\mathbf{m}'}^{11}(\tau) = -4\langle \hat{P}T_{\tau}a_{\mathbf{m}}(0)a_{\mathbf{m}'}^{+}(\tau)f_{\mathbf{m}'}^{+}(\tau)f_{\mathbf{m}'}(\tau)\rangle$$

are the corresponding two-particle Green's functions. A few diagrams used to calculate these Green's functions are

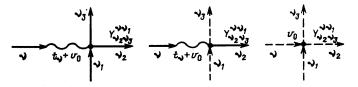


FIG. 1. Bare interaction vertices.

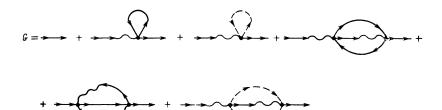


FIG. 2. Several first-order diagrams for the boson Green's function (the dotted lines denote the fermion Green's function F).

shown in Fig. 4. Repeating the entire procedure of converting from the lattice site representation to the representation (15) for the bipolaron Green's function, and using the diagonal property discussed in the Appendix, we obtain an expression similar to the one derived in Ref. 8:

$$G_{\mathbf{v}}^{b}(\boldsymbol{\omega}_{j}) = [1 - 2n_{b} + A_{\mathbf{v}}(\boldsymbol{\omega}_{j})] G_{\mathbf{v}}(\boldsymbol{\omega}_{j}), \qquad (23)$$

where the strength operator $A_{\nu}(\omega_j)$ is a sum of diagrams starting with the third diagram (Fig. 4). Expression (23) shows that the spectrum of excitations is entirely determined by the Bose functions.

In calculating the diagrams for the bipolaron Green's function, we encounter vertices associated with the presence of three operators all evaluated at the same instant of time and space. A factor $-v_c Y_{\nu\nu_1}^{\nu_2\nu_3}$ (where ν_2 , ν_3 refer to the outgoing vertices and ν , ν_1 refer to the incoming vertices) is associated with such a vertex in G^{II} , while a factor of $-2v_c Y_{\nu\nu_1}^{\nu_2\nu_3}$ is associated with an F^{II} vertex of this kind.

2. CRITICAL MAGNETIC FIELD OF A CONDENSATE OF SMALL BIPOLARONS FOR ARBITRARY CONCENTRATIONS

As we noted above, the energy spectrum can be determined completely once the Bose Green's function, which will be discussed below, is known. The diagrammatic series for the self-energy part Σ_{v} (ω_{j}) can be conventionally divided into two groups of terms: the first group consists of diagrams that allow us to isolate the strength operator A_{v} (ω_{j}), while the second consists of all the remaining diagrams (e.g., the fourth diagram in Fig. 2). A similar division allows us to write the Dyson equation for G_{v} (ω_{j}):

$$G_{v}^{-1}(\omega_{j}) = i\omega_{j} + t_{v} - [2n_{b} - A_{v}(\omega_{j})](t_{v} + v_{o}) - \Sigma_{v}(\omega_{j}) + \mu. \quad (24)$$

Since we are discussing the band edge, the bare spectrum can be written as follows:

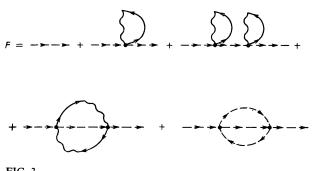


FIG. 3.

 $\varepsilon_{v} = -\mu - t_{0} + (p_{2}^{2}/2m^{**}) [1 - 2n_{b} + A_{0}(0)].$

In analogy with Ref. 7, let us write the Bose Green's function for the lowest Landau level in the neighborhood of the phase transition [i.e., for $T \gtrsim T_c(H)$] in the following way:

$$G_{p_z}^{-1}(0) = J |p_z|^{\sigma} + \mu', \quad \sigma < 1,$$
(25)

where $\mu' = \mu + t_0 - [2n_b - A_0(0)](t_0 + v_0) - \Sigma_0(0)$ is the renormalized chemical potential and

$$J|p_{z}|^{\sigma} = (t_{0}+v_{0}) [A_{p}(0) - A_{0}(0)] + \sum_{p_{z}} (0) - \sum_{0} (0)$$
(26)

is the renormalized spectrum.

In the lowest Landau level, the fundamental contribution to the renormalization of the energy spectrum for the boson Green's function comes from the region of small momenta p_z . In this case the kinematic interaction may be treated as pointlike, so that we may replace t_v by t_0 . In order to solve Eq. (26) we will isolate that collection of diagrams in the self-energy part $\sum_{p_z} (0)$ that can be split into two parts joined by three boson Green's functions with $\omega_j = 0$, n = 0. If we do not include vertex corrections, summing these diagrams leads to the following equation:

$$\Sigma_{p_{z}}(0) = 4T^{2} v_{n}^{2} (t_{0} + v_{0})^{2} \sum_{v_{1} v_{2} v_{3}} |Y_{v_{2} v_{3}}^{vv_{1}}|^{2} G_{p_{z1}}(0) G_{p_{z2}}(0) G_{p_{z3}}(0).$$
(27)

Using the expression derived in the Appendix for calculating $\sum_{\nu_1\nu_2\nu_3} |Y_{\nu_2\nu_3}^{\nu\nu_1}|^2$, we obtain the following equation for the selfenergy part at small momenta in the lowest Landau level:

$$\Sigma_{r_{z}}(0) - \Sigma_{0}(0) = 2T^{2}g^{2} \int_{-\infty}^{\infty} \frac{dp_{z1} dp_{z2}}{\varepsilon_{p_{z1}}\varepsilon_{p_{z2}}} \left(\frac{1}{\varepsilon_{p_{z1}+p_{z2}+p_{z}}} - \frac{1}{\varepsilon_{p_{z1}+p_{z2}}}\right), \quad (28)$$

where $g^2 = v_c^2 (t_0 + v_0)^2 / l^4 (2\pi)^4$. For small momenta $p_z \ll a^{-1}$ the region of integration can be extended to infinity. In Eq. (28) ε_k is the renormalized spectrum. Exactly the same contributions give a result for $A_v(0)$ analogous to (28). The renormalized energy spectrum (26) is found from the nonlinear integral equation:

$$J | p_{z} |^{\sigma} = 4T^{2}g^{2} \int_{-\infty}^{\infty} \frac{dp_{z1} dp_{z2}}{\varepsilon_{p_{z1}}\varepsilon_{p_{z2}}} \left(\frac{1}{\varepsilon_{p_{z1}+p_{z2}+p_{z}}} - \frac{1}{\varepsilon_{p_{z1}+p_{z2}}} \right).$$
(29)

The solution to equations of this kind, which were discussed in the review article Ref. 7, is sought in the form

$$g^b = \left(\circ + \right) + \left(+ \right$$

FIG. 4.

 $\varepsilon_p = J |p|^{\sigma} + p^2/2\tilde{m}$, where $\tilde{m} = m^{**}/[1 - 2n_b + A_0(0)]$ is the renormalized bipolaron mass.

The upper critical magnetic field is determined from the condition that a Bose condensate of bipolarons forms, corresponding to vanishing of the renormalized chemical potential $\mu' = 0$ in the Bose Green's function $G_v(0)$. It is simpler to compute $H_{c2}(T)$ from the equation for the total number of bipolarons obtained from Eqs. (23) and (24):

$$n_{b} = -\mathcal{T} \sum_{\mathbf{v},\boldsymbol{\omega}} \frac{1 - 2n_{b} + A_{\mathbf{v}}(\boldsymbol{\omega}_{j})}{i\omega_{j} + t_{\mathbf{v}} - [2n_{b} - A_{\mathbf{v}}(\boldsymbol{\omega}_{j})](t_{\mathbf{v}} + v_{0}) - \Sigma_{\mathbf{v}}(\boldsymbol{\omega}_{j}) + \mu}.$$
(30)

Equations (29) and (30) allow us to determine the spectrum and the critical field. In order to make the problem easier, we distinguish the term with $\omega_j = 0$ and n = 0 from the sum (30); since we may assume $eH/m^{**}T \leq 1$, we can replace the rest of the sum by an integral. In this case it is convenient to rewrite Eq. (30) in the form

$$n_b - n_b^{c}(T) = T \sum_{p_x, p_z} \frac{1 - 2n_b + A_{p_z}(0)}{\varepsilon_{z}}, \qquad (31)$$

where $n_b^c(T)$ is the critical concentration of bipolarons at the temperature T.

For small momenta p_z the strength operator $A_{p_z}(0)$ does not have any sharp singularities; summing over p_x , we obtain

$$n_{b} - n_{b}^{\circ}(T) = T \frac{v_{\pi}}{\pi^{2}} eH[1 - 2n_{b} + A_{0}(0)] \int_{-\infty}^{\infty} \frac{dp_{z}}{|p_{z}|^{2}/2\tilde{m} + J||p_{z}||^{4}}.$$
(32)

From Eqs. (32) and (30) it is easy to find J and H_{c2} :

$$H_{c2}(T) = 0,26 \Phi_{0} \left(\frac{t_{0} + v_{0}}{m^{*}} \right)^{\frac{1}{2}} \frac{1}{v_{C}} \frac{\left[n_{b} - n_{b}^{c}(T) \right]^{\frac{1}{2}}}{T\left[1 - 2n_{b} + A_{0}(0) \right]}$$
$$J = 0,73 \left[\frac{(v_{0} + t_{0})^{3}}{m^{*}} \right]^{\frac{1}{2}} \frac{\left[n_{b} - n_{b}^{c}(T) \right]^{\frac{1}{2}}}{\left[1 - 2n_{b} + A_{0}(0) \right]^{\frac{1}{2}}}$$
(33)

where Φ_0 is the magnetic flux quantum.

Within the framework of the ladder approximation, the strength operator $A_0(0)$ entering into Eq. (33) can be described in the following way:

$$A_{0}(0) = 2T^{2}v_{C}^{2}(t_{0}+v_{0})\sum_{\substack{\nu_{1}\nu_{2}\nu_{2}\\\omega_{j}\omega_{j}'}}|Y_{\nu_{2}\nu_{2}}^{0\nu_{1}}|^{2}G_{\nu_{1}}(\omega_{j})G_{\nu_{2}}(\omega_{j}')G_{\nu_{2}}(\omega_{j}+\omega_{j}'),$$

where $G_{\nu_i}(\omega_j)$ is the renormalized Green's function (25). The fundamental contribution to the sum comes from terms with $\omega_j = \omega'_j = 0$. However, in contrast to the integral equation that determines the spectrum, in the limit $J(2\tilde{m}J)^{1/3} \ll 2eH/m^{**} \ll T$ under consideration here it is not correct to neglect all but the zero Landau level in this sum.

In these results the overlap integral acts as an interaction constant for the particles in the limit $v_0 \ll t_0$; in addition, this overlap integral determines the kinetic energy of the bipolarons and accordingly the Bose condensation temperature. In Ref. 5 it was shown within the random phase approximation that $n_b^c(T)$ has a temperature dependence that differs from the corresponding dependence for an ideal Bose gas, and under conditions where the dynamic interaction is absent we have for the critical temperature

$$T_c = tf(n_b)$$
.

Taking into account the expression for the effective mass $m^{**} = 1/2ta^2$, we can write the expression for H_{c2} for the case of a cubic lattice in the form

$$H_{c2}(T) = H_0 \frac{[1 - n_b^{\circ}(T)/n_b]^{\prime h}}{T/T_c},$$
(35)

where

$$H_0 = 0.45 \frac{\Phi_0}{a^2} \frac{n_b^{\eta_b}}{f(n_b)} \frac{1}{1 - 2n_b + A_0(0)}$$

Let us now discuss the upper critical field for the case of small bipolaron concentrations. In this limit $n_b^c(T)$ and $f(n_b)$ can be replaced by the corresponding expressions for an ideal Bose gas:

$$n_b^{\circ}(T)/n_b = (T/T_c)^{\eta_b}, \quad f(n_b) = 6.62 n_b^{\eta_b}, \quad n_b \ll 1.$$

For small concentrations the strength operator satisfies $A_0(0) \sim n_b^{4/3}$ and, consequently, we may neglect it. As a result, we obtain for H_0

$$H_0=0.14 \frac{\Phi_0}{a^2} \frac{n_b^{*/0}}{1-2n_b}$$

3. DISCUSSION

(34)

Since no condensate forms in an ideal charged Bose gas in the presence of a magnetic field, in our previous papers^{6,7} we have studied systems of bosons with various types of interactions.

Reference 6 contains a discussion of a charged Bose gas interacting with impurities in the lattice. It was found that the presence of defects causes smearing of the Landau levels and elimination of the quasi-one-dimensional singularity in the density of states, which in turn leads to nonzero $H_{c2}(T)$. The quantity $H_{c2}(T)$ calculated in Ref. 6 had the following form:

$$H_{c2}(T) = 2.24 \frac{\Phi_0}{\chi^{\eta_0} l_0^{\eta_0}} \left[\frac{1 - (T/T_c)^{\eta_0}}{T/T_c} \right]^{\eta_0} , \qquad (36)$$

where $\lambda = 2\pi (2m^{**}T_c)^{-1/2}$ is the de Broglie wavelength and l_0 is the mean-free path of the particles.

Reference 7 contains a discussion of a charged Bose gas in which the Coulomb interaction between bosons is screened; this allowed us to treat the interaction as shortrange. In this case elimination of the quasi-one-dimensional singularity for the lowest Landau level is a result of renormalization of the energy spectrum, as it is in the analysis presented here. This leads to a temperature dependence $H_{c2}(T)$ similar to (36):

$$H_{c2}(T) = 0.18 \Phi_{\rm e} m^{..} T_{\rm e} \eta^{..} \frac{\left[1 - (T/T_{\rm e})^{..}\right]^{..}}{T/T_{\rm e}}, \qquad (37)$$

where

 $\eta = m^{\prime\prime} n^{\prime\prime_3} v_0 / 4\pi.$

In this paper we have investigated a system of small singlesite bipolarons for arbitrary average bipolaron concentrations per unit cell. We have shown that in all concentration regions the bipolaron Green's function may be expressed in terms of a boson Green's function, and we have also calculated the upper critical field H_{c2} when the dynamic interaction is absent. Our results prove that the difference between bipolaron statistics and boson statistics gives rise to the existence of a finite critical field even in the absence of bipolaron-bipolaron interactions.

Despite the differing interaction mechanisms, the functions $H_{c2}(T)$ given in (33), (36) and (37) share certain general features:

(1) they are all nonlinear near the critical point T_c : specifically, $H_{c2}(T) \propto (T_c - T)^{3/2}$;

(2) they all possess positive curvature.

In addition, the critical fields (33), (36) and (37) all depend on the interaction constant in a similar fashion. The general properties of these systems indicate that the temperature dependence of H_{c2} is determined by the type of statistics, and consequently the type of phase transition, and not the form of the interaction in a quantizing magnetic field.

The functions $H_{c2}(T)$ we have obtained differ both from those calculated within the mean-field approximation, i.e., $H_{c2}^{\text{mf}} \propto T_c - T$, and those calculated by using a phenomenological functional that takes fluctuations into account, i.e., $H_{c2}^{\text{fl}} \propto (T_c - T)^{4/3}$. Since the superconductivity of bipolarons is analogous to superfluidity in He⁴, we might expect that the region of applicability of the mean-field approximation will be small. The results obtained in this paper are valid within the temperature range $(1 - T/T_c)^{1/2} \ge 0.05 n_b^{1/6}$ [for (37) we have $1 - T/T_c \ge 0.03\eta$; see Ref. 7], which is interrupted by a region in which fluctuations play a significant role. Therefore, as a function of anisotropy and the interaction of the bipolarons, the function $H_{c2}(T)$ observed in reality may be described in the following way:

(1) in the immediate vicinity of T_c we have the function $H_{c2}^{f1}(T)$, which changes into $H_{c2}(T) \propto (T_c - T)^{3/2}$ as the temperature decreases;

(2) in the intermediate temperature range we have yet another function $H_{c2}^{mf}(T)$. In what follows we will discuss and evaluate the experimental data concerning the upper critical field of the metallic oxides.

All the high-temperature superconductors discovered

to date, with the exception of the recently discovered KBaBiO, exhibit strong anisotropy between the *ab* planes and the *c* axis.⁹⁻¹¹ By repeating all the calculations presented here with the approximation of an anisotropic effective mass, we may obtain the following expression for H_0 :

$$H_{0}=0.4\frac{\Phi_{0}}{v_{c}}\left(\frac{t_{0}+v_{0}}{m_{H}}\right)^{\frac{1}{2}}\frac{n_{b}^{u_{h}}}{T_{c}\left[1-2n_{b}+A_{0}(0)\right]},$$

where m_H^{**} is the effective mass of a bipolaron in the direction of the magnetic field, $m_H^{**} = (m_{\parallel}^{**}\cos^2\theta + m_1^{**}\sin^2\theta)$, and θ is the angle between the *c* axis and the direction of the magnetic field; the labels $\langle \langle 1 \rangle \rangle$ and $\langle \langle \parallel \rangle \rangle$ denote values along the *c* axis and in the *ab* plane. In this model the overlap integral satisfies $t_0 = 2t_{\parallel} + 4t_1$. In what follows we will assume $t_1 \gg t_{\parallel}$, which follows from the strong anisotropy that is observed in the experimental measurements of the field H_{c2} and the resistivity ρ of single crystals. The term $A_0(0)$ entering into these formulae can be estimated from expression (34), assuming that the basic contribution to this sum comes from eigenvalues in the region of large *n*, and $A_0(0)$ is found to be of order unity. The function $H_0(\theta)$ is conveniently written in a form that does not contain either the bipolaron overlap integral or the effective mass explicitly:

$$H_{0}(\theta) = H_{c2}^{\perp}(T) \left(\varepsilon^{2} \cos^{2} \theta + \sin^{2} \theta \right)^{-\gamma_{0}}, \qquad (38)$$

where $\varepsilon = (m_{\parallel}^{**}/m_{\perp}^{**})^{1/2}$. It is clear from expression (38) that within the approximations used here the angular dependence of H_{c2} is similar to $H_{c2}(\theta)$ calculated within the Landau-Ginzburg theory with anisotropic coherence lengths $\xi_{\parallel}, \xi_{\perp}$.^{12,13} In experimental measurements of the anisotropy of H_{c2} it is observed that 1^{12-15}

$$\epsilon = H_{c2}^{\perp}/H_{c2}^{\parallel} = 6 - 13.$$

In our estimate of the critical field H_{c2} we will use a value of the concentration of positive carriers equal to its measured Hall-effect value, i.e., $p = 6 \cdot 10^{21}$ cm⁻³, (Ref. 16). Then we have $n_b = pv_c/2 \sim 0.5$, and the lattice parameters satisfy $a_{\parallel} = 11.674$, $a_{\perp} = 3.891$ Å (in these compounds a and b differ by small amounts which may be neglected). Therefore, near T_c we obtain for H_{c2}^{\perp} (in tesla):

 $H_{c2}^{\perp}(T) \approx 10^{3} (1 - T/T_{c})^{\frac{4}{3}}.$ (39)

The first communications to appear in print on measurement of the critical magnetic field reported a low value for H_0 , linear growth near T_c and a weak positive curvature (see, for example, Refs. 10 and 17). Subsequent measurements of H_{c2} in rather good single crystals come close to the absolute magnitude of H_0 given by Eq. (39), e.g., $H_0 = 700$ T for YBa₂Cu₃O_{7-x} (Ref. 14), 300 T for (Ho, Gd) Ba₂Cu₃O_{7-x} (Ref. 13), 810 T for EuBa₂Cu₃O_{7-x} (Ref. 15), etc.

By now the number of reasonably plausible experiments is large enough to allow us to recognize certain distinctive features in the behavior of the new high-temperature superconductors [including more recent data on the compounds Tl-Ba-Ca-Cu-O (Ref. 18) and Bi-Sr-Ca-Cu-O (Ref. 19)] in a magnetic field.

(1) For all the anisotropic hole-doped metallic oxides the resistive transition does not shift when a magnetic field is applied, in contrast to normal superconductors; although the transition is broadened, its beginning is almost unaffected by the field.

In contrast, for the system KBBO (Ref. 20), in which anisotropy is absent, the curve for the resistance $\rho(T)$ undergoes a parallel shift in a magnetic field as the field H increases, as in ordinary superconductors. In the strongly anisotropic electron-doped metallic oxide Nd_{2-x}Ce_xCuO_{4-x} (Ref. 21) both types of behaviors of $\rho(T)$ were observed, i.e., broadening of the dependence of $\rho(T)$ in a field H^{\perp} and a parallel shift in a field H^{\parallel} .

(2) Independent of the criterion for determining $T_c(H)$, the temperature dependence $H_{c2}(T)$ exhibits positive curvature.

(3) In the majority of papers^{9-15,19-23} a nonlinear increase was observed for $H_{c2}(T)$ near T_c . The measurement of the critical exponent ν , which is defined as the exponent in the power-law function $H_{c2}(T) \propto (1-\tau)^{2\nu}$, gives a scatter of values from 0.65 to 0.8. In this case the indices for H_{c2}^{\parallel} and H_{c2}^{\perp} are different: $2\nu_{\parallel} = 1.32$ from Ref. 12 and 1.3 from Ref. 14, while $2\nu_{\perp} = 1.48$ from Ref. 12 and 1.6 from Ref. 14.

Since the coherence length calculated from the BCS equations is small, $\xi_{\parallel} \sim 6$ Å, the region of fluctuations is considerably larger than in standard superconductors: $1 - T/T_c \sim (T_c/E_F)^4$. Using the phenomenological expression for the free energy which includes fluctuations, we can obtain $\nu = 2/3$ for the critical exponent.²⁴ The same result is also obtained for strongly localized electrons,²⁵ in which the superconductivity is similar to superfluidity in He⁴ (e.g., for bipolarons). The region of fluctuations ΔT_f for such systems is bounded:

$$|1-T/T_{c}| \sim \frac{1}{32\pi^{2}\Delta C\xi_{\parallel}^{3}} \sim 10^{-3},$$

this is confirmed by measurements of the behavior of the specific heat ΔC of the high-temperature superconductors near T_c [$\Delta T_f \approx 0.2$ K, $\nu = 0.75$ (Ref. 22)]. In Refs. 12 and 14 the measurements were carried out up to rather large fields of about 20 T, and over a large temperature range up to 25 K $\gg \Delta T_f$.

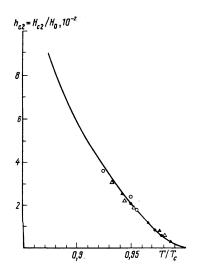


FIG. 5. Temperature dependence of the upper critical field h_{c2} near T_c : \blacktriangle —Ref. 23, O—Ref. 13, \bigtriangleup —Ref. 16, \blacklozenge —Ref. 12. In this experiment the field was perpendicular to the *c* axis.

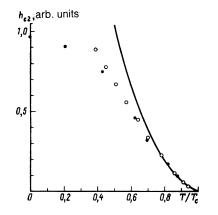


FIG. 6. Temperature dependence of the field h_{c2} for EuBa₂Cu₃O_{7-x} (Ref. 17) (\bullet is for the field parallel to the *c* axis and $H_0 = 30$ T) and for Ba_{0.63} K_{0.37} BiO₃ (Ref. 20) (\bigcirc is for H = 9 T); the solid line is the theoretical curve (35).

Although anisotropy can broaden the region of fluctuations, the critical exponent cannot be larger than 2/3 in this theory. In the experiments, however, a rather large region was observed with $H_{c2} \propto (1 - T/T_c)^{3/2}$ (see Fig. 5). From this we see that the observed nonlinear dependence of H_{c2} cannot be explained by the influence of fluctuations. The decrease in the value of 2ν to 1.3 in the direction of the c axis can be explained either by twinning [which leads to a dependence $H_{c2}^{\parallel} \propto (T_c - T)^{1/2}$ (see Ref. 26)], or by an enlarged region of applicability of the mean-field approximation. Furthermore, the quasi-one-dimensionality of the bipolarons in a magnetic field leads to the possibility of bipolaron localization, especially along the c direction, where the overlap integral t_{\parallel} is small. Apparently, the low value of H_{c2}^{\parallel} found in Ref. 15 for the compound $EuBa_2Cu_3O_{7-x}$ is connected with this (Fig. 6).

Because of the large critical fields H_{c2} we did not succeed in mapping out the entire curve $H_{c2}(T)$. Figure 6 shows an almost complete profile of H_{c2} for EuBa₂Cu₃O_{7-x} and KBBO, and the theoretical curve $H_{c2}(T)$. The lack of agreement between the experimental points and the calculated curve apparently is due to the poor coupling between the layers in the direction of the *c* axis, which corresponds to a function $\rho(T)$ of semiconductor type.¹⁵

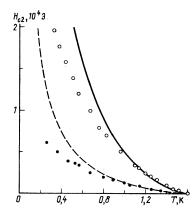


FIG. 7. Comparison of the experimental²⁷ and theoretical functions $H_{c2}(T)$, the latter from (37), for $\text{Li}_{0.9} \text{Mo}_6 \text{O}_{11}$ for cases where the field is perpendicular (O) and parallel (\bullet) to the *c* axis.

Note that unusual behavior of $H_{c2}(T)$ has been observed previously, e.g., in the low-temperature anisotropic metallic oxide $Li_{0.9}Mo_6O_{17}$, (Ref. 27), where agreement with our theoretical curve is better (Fig. 7).

If we assume that the same sort of superconductivity exists in the systems KBBO, Y (RE)BCO, NCOO, TBCCO, etc., the similar behavior of the curves $H_{c2}(T)$ cannot be due either to the layer-like structure or to broadening of the region of fluctuations.

APPENDIX

In calculating the bipolaron Green's function we have used the diagonal property of the self-energy part Σ_{v} in (24) and the strength operator A_{y} in (23). Consider an arbitrary diagram of order N for the self-energy part which contains both pointlike dynamic interactions and the kinematic interaction t_{y} :

 $\Sigma_{\nu\nu'}(\omega_j)$ $= \sum_{\substack{\mathbf{v}_1...\mathbf{v}_{2N-1}\\ \boldsymbol{\omega}_{j1}...\boldsymbol{\omega}_{jN}}} Y_{\mathbf{v}_i\mathbf{v}_i}^{\mathbf{v}\mathbf{v}_1} \dots Y_{\mathbf{v}_{2N-1}\mathbf{v}'}^{\mathbf{v}_{2N-3}\mathbf{v}_{2N-2}} G_{\mathbf{v}_i}^0(\boldsymbol{\omega}_{j1}) \dots G_{\mathbf{v}_{2N-1}}^0(\boldsymbol{\omega}_{jN})$ $\times (t_{v_1} + v_0) \dots (t_{v_{2N-1}} + v_0).$ (A1)

Since G_v^0 and t_v depend only on p_z and n, let us separate out the sum over p_{x_i} . It is clear from (16) that at each vertex Y the law of conservation of the momenta p_x and p_z is fulfilled, and consequently

$$\Sigma_{vv'} = \Sigma_{p_{z,nn'}} \delta_{p_{z}p_{z'}} \delta_{p_{x}p_{x'}}.$$

Making use of the definition (16), we can sum over all the momenta p_{x_i} and obtain

$$\Gamma^{\mathbf{v}\mathbf{v}'} = \sum_{p_{\mathbf{x}1},\dots,p_{\mathbf{x}2N-1}} Y_{\mathbf{v}_{\mathbf{x}}\mathbf{v}_{\mathbf{s}}}^{\mathbf{v}_{\mathbf{v}_{1}}}\dots Y_{\mathbf{v}_{2N-1}\mathbf{v}'}^{\mathbf{v}_{2N-2}} \\
= \int \frac{dx_{1}\dots dx_{N} dy_{1}\dots dy_{N}}{l^{2N-1} (2^{n+n'} n! n'!)^{1/s}} \\
\times \chi_{n, p_{\mathbf{x}}}(x_{1}, y_{1}) \chi_{n', p_{\mathbf{x}}}(x_{N}, y_{N}) \prod_{\{l, m\}} I_{l, m}(x_{l}, x_{m}, y_{l}, y_{m}),$$
(A2)

where x_i is the coordinate of the *i*th vertex (nondimensionalized by l),

$$I_{lm}(x_{l}, x_{m}, y_{l}, y_{m}) = \exp\left[-\frac{i}{2}(x_{m}-x_{l})(y_{m}+y_{l})\right]$$

$$\times \exp\left[-\frac{(y_{m}-y_{l})^{2}+(x_{m}-x_{l})^{2}}{4}\right]L_{u_{lm}}\left[\frac{(y_{m}-y_{l})^{2}+(x_{m}-x_{l})^{2}}{2}\right],$$

 $L_{n_{lm}}$ is a Laguerre polynomial, and the product is extended over all lines that connect the l th vertex to the *m*th. Let us pass to a new system of coordinates:

328 Sov. Phys. JETP 72 (2), February 1991 Then taking into account that the number of incoming and outgoing lines is the same at each vertex except the Nth, in the new coordinates we obtain:

$$\prod_{\{l,m\}} I_{lm}(x_{l}, x_{m}, y_{l}, y_{m}) = \exp\left[-\frac{i}{2}\left(x_{N}'y_{N}' - \frac{2x_{N}'}{N}\sum_{i}y_{i}'\right)\right] \\ \times \exp\left[-\frac{i}{2}\sum_{\{l,m\}} (x_{l1}'y_{m1}' - x_{m1}'y_{l1}')\right] \\ \times \prod_{\{l,m\}} \exp\left(-\frac{(y_{m1}' - y_{l1}')^{2} + (x_{m1}' - x_{l1}')^{2}}{4}\right) \\ \times L_{n_{lm}}\left(\frac{(y_{m1}' - y_{l1}')^{2} + (x_{m1} - x_{l1})^{2}}{2}\right).$$

The expression given here does not contain x'_1 ; therefore, we can integrate over x'_1 and evaluate the following integral over y'_1 :

$$[l^{2N}(2^{n+n'}n!n'!)^{\frac{1}{2}}(2\pi)^{2N-\frac{1}{2}}]^{-1} - \frac{1}{N} \int_{-\infty}^{\infty} dy_{1}' \exp[ip_{x}lx_{N}' - p_{x}^{2}l^{2} - p_{x}l(y_{1}'+y_{N}')]$$
$$\times H_{n}(y_{1}'+p_{x}l)H_{n'}(y_{N}'+p_{x}l)\exp\left[-\frac{(y_{1}'+y_{N}')^{2}}{2}\right].$$

2

Let us make the substitution

$$\xi = \frac{1}{N} \sum_{i}^{N} y_{i}' - \frac{y_{N}'}{2}$$

which finally leads to

$$\left(\frac{2^{n+1}n!}{2^{n'}n'!}\right)^{\nu_{1}} \frac{1}{l^{2N}} \frac{1}{(2\pi)^{2N-1}} \exp\left(-\frac{y_{N}'^{2} + x_{N}'^{2}}{4}\right)$$
$$\times (y_{N1}' + ix_{N1}')^{n'-n} L_{n}^{n'-n} \left(\frac{y_{N}'^{2} + x_{N}'^{2}}{2}\right), \quad n \le n'.$$
(A3)

In the remaining part of the integral (A2) we will pass to polar coordinates

$$x_{k1}' = \rho_{k1} \cos \varphi_k, \quad y_{k1}' = \rho_{k1} \sin \varphi_k$$

and obtain the following expression:

$$\int \rho_{21} d\rho_{21} \dots \rho_{N1} d\rho_{N1} d\phi_{2} \dots d\phi_{N}$$

$$\times \prod_{\{l,m\}} F_{lm}(\rho_{l1}, \rho_{m1}, \cos(\varphi_{l1} - \varphi_{m1}))$$

$$\times \exp\left(-\frac{\rho_{N1}^{2}}{4}\right) \rho_{N1}^{n'-n} \exp\left[i(n'-n)\varphi_{N}\right] L_{n}^{n'-n}\left(\frac{\rho_{N1}^{2}}{2}\right)$$

$$\times \exp\left[-\frac{i}{2} \sum_{\{l,m\}} \rho_{l1}\rho_{m1} \sin(\varphi_{l} - \varphi_{m})\right]. \quad (A4)$$

For lines that connect the *l* th vertex to the first vertex, we have

$$F_{li} = L_n \left(\frac{\rho_l^2}{2} \right) \exp \left(- \frac{\rho_l^2}{4} \right).$$

With the help of the change of variables

 $\tilde{\varphi}_2 = \varphi_2 - \varphi_N, \ldots, \varphi_{N-1} = \varphi_{N-1} - \varphi_N$

we can integrate (A4) with respect to φ_N and obtain

$$\Gamma^{\nu\nu'} \sim \delta_{\nu\nu'}, \quad \Sigma_{\nu\nu'}(\omega_j) = \Sigma_{\nu}(\omega_j) \delta_{\nu\nu'}. \tag{A5}$$

- ¹J. C. Bednorz and K. A. Muller, Z. Phys. B 64, 189 (1986).
- ²J. Ashburn, C. J. Torng, C. W. Chu *et al.*, Phys. Rev. Lett. **58**, 908 (1987).
- ³A. S. Aleksandrov, Pis'ma Zh. Eksp. Teor. Fiz. **47**, 642 (1987) [JETP Lett. **47**, 737 (1988)].
- ⁴A. S. Aleksandrov, Pis'ma Zh. Eksp. Teor. Fiz. **46** (Appendix), 128 (1987) [JETP Lett. **46**, 160 (1987)].
- ⁵A. Aleksandrov and J. Ranninger, Phys. Rev. B 23, 1796 (1981); Phys. Rev. 24, 1164 (1981).
- ⁶A. Aleksandrov, J. Ranninger, and S. Robaszkiewicz, Phys. Rev. B 33, 4526 (1986).
- ⁷ A. Aleksadrov, D. A. Samarchenko, and S. V. Traven', Zh. Eksp. Teor. Fiz. **93**, 1007 (1987) [Sov. Phys. JETP **66**, 567 (1987)].
- ⁸V. G. Bar'yakhtar V. I. Krivoruchko, and Yablonskii, Preprint ITF-82-148P (Inst. Theor. Phys.), USSR Acad. Sci.
- ⁹O. Laborde, J. L. Tholence, P. Lejay et al., Solid State Commun. 63, 915 (1987).

- ¹⁰ T. K. Worthington, W. J. Gallagher, and T. R. Dinger, Phys. Rev. Lett. **59**, 1160 (1987).
- ¹¹ N. J. Naughton, P. M. Chaikin, C. E. Chu *et al.*, Phys. Rev. Lett. **62**, 531 (1987); J. M. Tarascon, L. H. Greene, and P. Barboux, Phys. Rev. B **36**, 8393 (1987).
- ¹² T. K. Worthington, W. J. Gallagher, and D. L. Caiser, Physica C 153-155, 32 (1988).
- ¹³ Y. Iye, T. Tamegai, T. Sakalibara et al., Physica C 153–155, 26 (1988).
- ¹⁴ B. Oh, A. Kapitulik, K. Char, Phys. Rev. B 37, 7861 (1988).
- ¹⁵ Y. Tajima, M. Hikita, T. Ishii *et al.*, Phys. Rev. B 37, 7956 (1988).
 ¹⁶ I. G. Gorlov, Pis'ma Zh. Eksp. Teor. Fiz. 47, 578 (1988) [JETP Lett.
- 47, 672 (1988)].
- ¹⁷ K. Takita, H. Akinaga, H. Katoh *et al.* Jpn. J. Appl. Phys. 26, L1552 (1987).
- ¹⁸ H. Kumakura, K. Togano, K. Takahashi et al., Jpn. J. Appl. Phys. 27, L857 (1987).
- ¹⁹ J. Beille, H. Dupendant, O. Laborde et al., Physica C 156, 448 (1988).
- ²⁰ U. Welp, W. K. Kwok, G. W. Crabtree et al., Physica C 156, 27 (1988).
- ²¹ Y. Hidaka and M. Suzuki, Nature 338, 635 (1989).
- ²² D. H. Ginsberg, S. E. Inderhees, M. B. Salamon *et al.*, Phys. Rev. B 38, 885 (1988).
- ²³ O. Laborde, P. Monceau, and M. Potel, Physica C 153-155, 1467 (1988).
- ²⁴ M. L. Kulic and H. Stenschke, Physica C 153-155, 679 (1988).
- ²⁵ V. L. Ginzburg, A. A. Sobyanin, and L. I. Bulaevskii, Zh. Eksp. Teor. Fiz. **94**(7), 355 (1988) [Sov. Phys. JETP **67**, 1499 (1988)].
- ²⁶ L. A. Schwartzkopf, M. M. Fang, L. S. Chumbley *et al.*, Physica C 153– 155, 1463 (1988).
- ²⁷ C. Schlenker, H. Schwenk, J. Markus *et al.*, Physica B + C **135**, 511 (1985).

Translated by Frank J. Crowne