The mechanism for superconductivity in doped fullerite A_xC_{60}

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It is shown that the high symmetry of both the C_{60} molecules themselves and also of the fcc crystal lattice lies at the basis of the "high-temperature" superconductivity of C_{60} fullerene doped with alkali metal atoms and thallium. The first causes the dynamic Jahn–Taller effect when the electrons interact with the intramolecular vibrations of the fullerene C_{60}, while the second produces a multi-valley conduction band and a multiply connected Fermi surface when the doped fullerite has the stoichiometric composition A_3C_{60} ($A = K,Rb,Cs$). Both factors contribute to the raising of the electron–phonon coupling constant and, as a consequence, to the increase in the critical temperature T_c of the superconducting transition in A_3C_{60} (or $RbTl_2C_{60}$), unlike solid hyperfullerenes C_n for $n \geqslant 70$ with lower molecular and lattice symmetry.

1. INTRODUCTION

The sensational discovery by Hebard *et al.*[1] of superconductivity in the crystal phase of the new allotropic form of carbon, fullerene C_{60} (Ref. 2) with fairly high superconducting (SC) transition temperatures, T_c being ≈ 20–30 K on doping with alkali metals[3–5] and even ≈ 48 K in the compound $RbTl_2C_{60}$ (Ref. 6) (see also review by Loktev[7]) raised the question of the nature of this phenomenon and its possible connection with the mechanism for high-temperature superconductivity (HTSC) in metallic compounds containing copper [LaBaCuO (Ref. 8), YBaCuO (Ref. 9), BiSrCaCuO (Ref. 10), TlBaCaCuO (Ref. 11)], and also without copper [BaKBiO (Ref. 12)].

The extremely rich vibrational spectrum of C_{60} molecules and correspondingly the phonon spectrum of crystalline fullerene–fullerite extending to frequencies $\omega \approx 2 \cdot 10^3$ cm^{-1} (Ref. 13), and also the effects of raising T_c as the radius of the dopant atoms[14] increases and lowering it as the pressure increases[15] shows that the basis of the superconductivity of doped fullerite A_xC_{60} ($A = K,Rb,Cs$) is most likely the Cooper pairing of conduction electrons due to the electron–phonon interaction (EPI), i.e., the standard BCS mechanism.[16] In fact, the introduction of atoms (ions) with large radius (Cs,Tl) into the lattice of the molecular fullerite crystal causes it to expand and reduces the overlap of π-orbitals (p_z-orbitals) of neighboring C_{60} molecules, i.e. reduces the width of the conduction band and causes the density of states (DS) at the Fermi level $N(0)$ to grow, and consequently increases the EPI constant $\lambda_{ph} = N(0)\ g^2_{ph}$ and raises T_c (Refs. 7, 14). High hydrostatic pressure[15] produces the opposite effect: it increases the overlap of the π-orbitals, broadening the conduction band, reducing the DS and the constant λ_{ph}, and hence reducing T_c. It then remains unclear why superconductivity is absent (or, in any case, strongly suppressed) in A_3C_{70} and $A_3(C_{60})_{1-y}(C_{70})_y$ crystals (Ref. 17), the phonon spectra of which are even richer.

Other suggestions made up to the present, based on the EPI model (for example, a nonlinear bisoliton model of interaction with acoustic phonons[18] or EPI models with low- and high-frequency phonons[19,20]) do not give an answer to this problem; essentially they do not reflect any individual features of crystals based on C_{60} fullerene which favor a SC transition compared with solid hyperfullerenes C_n with $n \geqslant 70$. A similar problem can also be posed in relation to the hypothesis proposed by Pietronero[21] about whether the EPI is amplified by a factor $(1 + \lambda_{ph})$ due to the phonon vertex renormalization (where λ is the dimensionless EPI constant $\bar{\omega}_{ph}$) in the case of sufficiently high phonon frequencies, exceeding the Fermi energy E_F of the electrons when the density of the latter is low. We note that in Ref. 21 to estimate the Coulomb repulsion the Morel–Anderson potential[22] was used without justification; its introduction is only valid for $\bar{\omega}_{ph} \ll E_F$, while for $\bar{\omega}_{ph} \gg E_F$ the constant of the Coulomb repulsion is not weakened because of the Bogolyubov–Tolmach logarithm.

It is shown in the present work (see also Loktev and Pashitskiĭ[23]) that the main reason for "high-temperature" superconductivity in doped fullerite with the stoichiometric composition A_3C_{60} is the high symmetry of both the C_{60} molecule (*buckyball*) and of the cubic fullerite crystal (with a fcc lattice), which leads on the one henad to the appearance of the dynamic Jahn–Teller effect and on the other to many-valley structure of the electron spectrum in the conduction band. Both these effects appreciably enhance the EPI and raise T_c in A_3C_{60}, but are absent in the solid phase of the C_{70} fullerene with lower molecular and lattice symmetry, in which superconductivity is not found in doping.[17]

2. DYNAMIC JAHN–TELLER EFFECT

Group theoretical analysis of the symmetry of electronic and electron-vibrational states of the highly symmetrical *buckyball* C_{60}, carried out in a large number of works,[24–27] reveals that nearly all states of this molecule are degenerate. However, filling of the sixty external π electrons of the lowest states leads to an electronic structure in some sense analogous to the closed shells of atoms of the inert elements, when the last (highest energy) state, namely the five-fold degenerate h_u state, is filled just like all the lower-lying states. This in turn is evidence that the ground-state many-electron configuration of the C_{60} molecule is nondegenerate and is consequently stable relatative to a change in its icosahedral shape, which is strictly confirmed by Y_h symme-

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try of C_{60} molecules, which is the highest possible among the point groups.

The first unfilled state t_{1u} of this molecule is threefold degenerate and can manifest itself either through electronic excitation of fullerene or through ionization. In both cases an electron term arises which according to the Jahn–Teller theorem is always unstable against lifting of the degneracy by deformation of the multiatomic molecule. The corresponding calculation using general group theory for a Y_h point group has already been carried out in the classic work by Jahn and Teller,[28] and specifically for all degenerate states of fullerene by Golod and Loktev.[24] It follows from this that h_g-symmetry strain vibrations are most strongly associated with the state t_{1u} which starts to fill up when fullerite is doped with monovalent alkali metals and neutral C_{60} molecules are transformed into partially ionized "molecular ions" (this was noted by Varma *et al.*[20]). Detailed numerical calculations carried out recently[29] confirm this conclusion and show that the largest EPI constants correspond to just the intramolecular Jahn–Teller h_g vibrations which also distinguish the C_{60} molecule among other fullerenes. On the other hand the D_{5h} symmetry of the C_{70} molecule is much lower and therefore essentially all representations are univariate and the degree of degeneracy does not exceed two. Therefore the Jahn–Teller effect cannot manifest itself in C_n molecules with $n \geqslant 70$, due to their relatively lower symmetry.

In the same way as the molecular state, the t_{1u} state also remains degenerate in the cubic crystal field of fullerene. This degeneracy is, however, partially lifted when one takes account of the migration of excess electrons between neighboring molecules due to the overlap of their π-orbitals, as a result of which a fairly narrow conduction band is formed (with a width less than 0.5 eV[29,30]), the filling of which, as a result of doping, transforms the dielectric C_{60} into a molecular metal A_xC_{60}. In agreement with many calculations, the s-states of the alkali metal atoms then give essentially no contribution to the state of the conduction band, which we also propose below. Strictly speaking, this conclusion, drawn in the majority of theoretical work (see Ref. 7) still requires deeper analysis, since a description of the metal-dielectric transition in the fullerite A_xC_{60} meets with some difficulty. In the model of the filling of the valence band this transition should occur for fairly small carrier concentrations x,[31] which is not confirmed by experiments which provide evidence that metal formation only takes place for $x \approx 3$ (Ref. 32).

We write the Hamiltonian describing the structure of the empty conduction band with one excess electron in the tight binding approximation in the form

$$H_{t_{1u}} = \varepsilon \sum_{\mathbf{n},\nu,\sigma} a^{+}_{\mathbf{n}\nu\sigma} a_{\mathbf{n}\nu\sigma} + \sum_{\mathbf{n},\mathbf{n}_1} \sum_{\substack{\nu,\nu_1\\ \sigma}} t^{\nu\nu_1}_{\mathbf{n}\mathbf{n}_1} a^{+}_{\mathbf{n}\nu\sigma} a_{\mathbf{n}\nu_1\sigma}, \tag{1}$$

where $\varepsilon = E(t_{1u}) - E(h_u)$ is the energy of the intramolecular electron transition from the h_u "ground" state to the first excited state t_{1u} of the C_{60} molecule, $a^{+}_{\mathbf{n}\nu\sigma}$ ($a_{\mathbf{n}\nu\sigma}$) is the creation (annihilation) operator for an electron with spin σ at the $\mathbf{n}$th site in the state ν from the t_{1u} multiplet, and $t^{\nu\nu_1}_{nn_1}$ is the overlap integral of different orbitals ($\nu \neq \nu_1$) of molecules in neighboring sites $\mathbf{n}$ and $\mathbf{n}_1$ of the fcc lattice. In the general case the diagonalization procedure for the Hamiltonian[1)] in the $\mathbf{k}$ representation is extremely cumbersome but it simplifies for certain directions of $\mathbf{k}$, for example, assuming $t^{\nu\nu_1}_{nn_1} = t_{nn_1}$ diagonals the band spectrum of the fcc crystal along the Brillouin zone (BZ) has the form

$$\varepsilon_{1,2}(\mathbf{k}) = \varepsilon - tz\gamma(\mathbf{k}), \quad \varepsilon_3(k) = \varepsilon + 2tz\gamma(\mathbf{k}), \tag{2}$$

where t is the value of t_{nn_1} for nearest neighbors, z is their number, and $\gamma(\mathbf{k})$ is the lattice structure factor. For $t > 0$ the minima (valleys) with high DS positioned on the BZ diagonal at the L-points, preserve the partial (two-fold) degeneracy, which agrees with numerical calculations.[26,30]

The interaction of the excess electron (or hole) with the vibrations responsible for the Jahn–Teller deformation of charged C_{60} molecules is described by the Hamiltonian

$$H_{\text{int}} = \sum_{\mathbf{n}} \sum_{\substack{\nu,\nu_1\\ \sigma}} \chi^{\nu\nu_1}_{\mathbf{n}} a^{+}_{\mathbf{n}\nu\sigma} a_{\mathbf{n}\nu_1\sigma} u^{\nu\nu_1}_{\mathbf{n}}, \tag{3}$$

where $\chi^{\nu\nu_1}_{\mathbf{n}}$ is the interaction matrix element mixing different components t_{1u} of the triplet in the molecule, while $u^{\nu\nu_1}_{\mathbf{n}}$ is the normal intromolecular vibration operator (in the general case there can be several such oscillations[29]) as a result of which $\chi^{\nu\nu_1}_{\mathbf{n}} \neq 0$ holds for $\nu \neq \nu_1$. As can be seen, in a pure fullerite (or in the stoichiometric compound A_3C_{60}) the interaction of Eq. (3) splits the fundamental degenerate band $\varepsilon_{1,2}(\mathbf{k})$ [see Eq. (2)] and thus induces an interband transition.

The use of the EPI Hamiltonian in the form of Eq. (3), on the assumption that the h_g symmetry vibrations of fullerene C_{60} are the most strongly interacting with the carriers, is substantiated by the results of experiments on inelastic neutron scattering.[13] According to the results obtained in that work h_g vibrations undergo the largest (both according to their position and also by the intensity of the corresponding lines in the neutron scattering spectra) change on going from the dielectric C_{60} fullerite crystal to the A_3C_{60} metal.

The existence of the Jahn–Teller modes in the vibrational spectrum of fullerene C_{60}, which are absent in the spectra of hyperfullerenes C_n ($n \geqslant 70$) with lower symmetry, should thus by itself bring about enhancement of the EPI and superconductivity in A_xC_{60} systems. On the other hand, the absence of superconductivity in the A_xC_{70} systems with a richer vibrational spectrum and with practically the same conductivity as in the normal phase of A_xC_{60} (Ref. 17) forces us to assume either an anomalously large value of the EPI constant with deformation Jahn–Teller modes or the existence of additional factors responsible for raising T_c in A_3C_{60}.

The role of such factors in the effective enhancement of the EPI could be played by the two-band electron spectrum of fullerite, associated with the dynamic splitting of the degenerate lower band $\varepsilon_{1,2}(\mathbf{k})$ and the many-valley structure of the conduction band which, according to numerical calculations,[25–27,30] consists in C_{60} fullerite of eight equivalent doubly degenerate minima (valleys at the L-points of the BZ and six deeper nondegenerate valleys at the X-points.

3. EFFECTS OF THE MULTIBAND (MULTI-VALLEY) NATURE OF A_3C_{60} AS A FACTOR IN RAISING T_c

The effective electron Hamiltonian of a metal with overlap at the Fermi level (FL) of partially filled bands or equivalent valleys in the BZ, i.e., with a multiply connected anisotropic Fermi surfaces (FS), in the **k** representation[33,34] has the form

$$H_{\text{eff}} = \sum_{\mathbf{k},t} \sum_{\sigma} [\varepsilon_i(\mathbf{k}) - \mu] a^+_{\mathbf{k}i\sigma} a_{\mathbf{k}i\sigma} + \sum_{\mathbf{k},\mathbf{k}_1,\mathbf{q}} \sum_{i,j,k,l} \sum_{\sigma,\sigma_1} W_{ij,kl} a^+_{\mathbf{k}+\mathbf{q}i\sigma} a^+_{\mathbf{k}_1-\mathbf{q}j\sigma_1} a_{\mathbf{k}_1 m\sigma_1} a_{\mathbf{k}l\sigma}, \tag{4}$$

where μ is the chemical potential determining the position of the FL, $a^+_{\mathbf{k}i\sigma}$ ($a_{\mathbf{k}i\sigma}$) is the creation (annihilation) operator of an electron with quasimomentum **k** and spin σ in the ith band (valley), and $W_{ij,kl}$ are the intra- and inter-band (inter-valley) interaction matrix elements, including the interaction of Eq. (3) (and also the EPI with all the remaining phonon branches) in second-order perturbation theory and with screened Coulomb repulsion.

If the FL intersects a doubly degenerate [see Eq. (2)] lower band, the degeneracy of which is lifted due to the EPI with constant $\chi^{\nu\nu_1}_{\mathbf{n}}$ ($\nu \neq \nu_1$), then the Gor'kov equations for the normal and anomalous Green's functions G_{ij} and F^+_{ij} ($i, j = 1,2$) in a two-band metal undergoing a SC transition take the form[33,34]

$$\begin{aligned} &[\omega - \xi_i(\mathbf{p})] G_{ij}(\mathbf{p}, \omega) + i\Delta_{ik}(\mathbf{p}, \omega) F^+_{kj}(\mathbf{p}, \omega) = \delta_{ij}, \\ &[\omega + \xi_i(\mathbf{p})] F_{ij}(\mathbf{p}, \omega) - i\Delta^+_{ik}(\mathbf{p}, \omega) G_{kj}(\mathbf{p}, \omega) = 0, \end{aligned} \tag{5}$$

where $\xi_i(\mathbf{p})$ is measured from the FL energy of electrons in the ith band (valley), and $\Delta_{ij}(\mathbf{p},\omega)$ is the anisotropic order parameter satisfying the self-consistency condition

$$\Delta_{ij}(\mathbf{p}, \omega) = \frac{1}{(2\pi)^4} \int d\mathbf{p}_1 d\omega_1 W_{ij,lm}(\mathbf{p}, \mathbf{p}_1, \omega - \omega_1) F_{lm}(\mathbf{p}_1, \omega_1). \tag{6}$$

When we take account only of the interband pairing of carriers[2)] in the logarithmic approximation we obtain in the limit $T \to T_c$ the following system of equations for the order parameters Δ_1 and Δ_2 in the dynamically split bands:

$$\begin{aligned} &\Delta_1 \left(1 - \Lambda_1 \ln \frac{\bar\omega_{ph}}{T_c}\right) - \Delta_2 \tilde\Lambda_{12} \ln \frac{\bar\omega_{ph}}{T_c} = 0, \\ &\Delta_2 \left(1 - \Lambda_2 \ln \frac{\bar\omega_{ph}}{T_c}\right) - \Delta_1 \tilde\Lambda_{12} \ln \frac{\bar\omega_{ph}}{T_c} = 0. \end{aligned} \tag{7}$$

Here

$$\Lambda_i = \lambda_i + \tilde\Lambda_{12}, \quad \tilde\Lambda_{12} = \Lambda_{12} + \tilde{\tilde\lambda}_{12}, \quad \Lambda_{12} = \frac{2\tilde\lambda^2_{12}}{1 - \lambda_{12} - \tilde{\tilde\lambda}_{12}}, \tag{8}$$

where $\lambda_i = N(0) W_{ii,ii}$ is the interband ($i = 1,2$) coupling constant, $\lambda_{12} = N(0) W_{12,12}$ is the direct interband coupling constant, $\tilde\lambda_{12} = N(0) W_{11,12} = N(0) W_{12,11}$ and $\tilde{\tilde\lambda}_{12} = N(0) W_{12,21} = N(0) W_{11,22}$ are constants describing one- and two-particle virtual interband transitions, and $\bar\omega_{ph}$ is the mean phonon frequency of the spectrum. We find from Eq. (7)

$$T_c = \bar\omega_{ph} \exp(-1/\tilde\Lambda), \tag{9}$$

where

$$\tilde\Lambda = \max \left\{ \frac{2(\Lambda_1 \Lambda_2 - \tilde\Lambda^2_{12})}{\Lambda_1 + \Lambda_2 \pm [(\lambda_1 - \lambda_2)^2 + 4\tilde\Lambda^2_{12}]^{1/2}} \right\}. \tag{10}$$

It follows from this, in particular, that for $\lambda_1 = \lambda_2 = \lambda > 0$ and $\Lambda_{12} > 0$ the effective coupling constant according to Eq. (8) is determined by the expression

$$\tilde\Lambda = \lambda + \tilde{\tilde\lambda}_{12} + 4\tilde\lambda^2/(1 - \lambda_{12} - \tilde{\tilde\lambda}_{12}) \tag{10a}$$

and can considerably exceed the EPI constant $\lambda = N(0) W$ in a single-band metal. It is possible that it is just for this reason that in A_3C_{60}, as a result of dynamic splitting of the conduction band under the action of strain vibrations of C_{60} molecules and the interband transitions induced by these vibrations, the SC state occurs with the fairly high value $T_c \gtrsim 20$ K. If $\tilde{\tilde\lambda}_{12} \sim \tilde\lambda^2_{12} \sim (\chi^{\nu\nu_1})^2$ (for $\nu \neq \nu_1$) is much larger than λ, then one should substitute the frequency of the "soft" Jahn–Teller mode, which can be appeciably less than $\bar\omega_{ph}$, as the pre-exponential multiplier in Eq. (9). Strong anharmonicity is then possible for the intramolecular vibration, showing up for example in the isotope-effect anomalies.[37,38]

Another factor which promotes the enhancement of the EPI and the raising of T_c is, as is well known,[39] the many-valley nature of the electron spectrum (multiconnected FS). When l equivalent valleys, filled with degenerate carriers exist, under the condition that the intra- and inter-valley momentum relaxation times are very different ($\tau_{ii} \ll \tau_{ij}$ for $i \neq j$) while intervalley scattering does not mix the states from different valleys in the time for Cooper pairing of electrons in a single valley, i.e., $\Delta_{ii}\tau_{ij} \gg 1$, but $\Delta_{ii}\tau_{ii} \ll 1$,[3)] the system of equations (5) including both intra- and inter-valley pairing ($\Delta_{ij} \neq 0$ for $i \neq j$) takes the form

$$\begin{aligned} &[\omega - \xi(\mathbf{p})] G(\mathbf{p}, \omega) + i\Delta(\mathbf{p}, \omega) F^+(\mathbf{p}, \omega) \\ &\qquad + i(l-1)\tilde\Delta(\mathbf{p}, \omega) \tilde F^+(\mathbf{p}, \omega) = 1, \\ &[\omega + \xi(\mathbf{p})] F^+(\mathbf{p}, \omega) - i\Delta^+(\mathbf{p}, \omega) G(\mathbf{p}, \omega) \\ &\qquad - i(l-1)\tilde\Delta^+(\mathbf{p}, \omega) \tilde G(\mathbf{p}, \omega) = 0, \\ &[\omega - \xi(\mathbf{p})] \tilde G(\mathbf{p}, \omega) + i\Delta(\mathbf{p}, \omega) \tilde F^+(\mathbf{p}, \omega) + i\tilde\Delta(\mathbf{p}, \omega) F^+(\mathbf{p}, \omega) \\ &\qquad + i(l-2)\tilde\Delta(\mathbf{p}, \omega) \tilde F^+(\mathbf{p}, \omega) = 0, \\ &[\omega + \xi(\mathbf{p})] \tilde F^+(\mathbf{p}, \omega) - i\Delta^+(\mathbf{p}, \omega) \tilde G(\mathbf{p}, \omega) - i\Delta^+(\mathbf{p}, \omega) G(\mathbf{p}, \omega) \\ &\qquad - i(l-2)\tilde\Delta^+(\mathbf{p}, \omega) \tilde G(\mathbf{p}, \omega) = 0, \end{aligned} \tag{11}$$

where the notation $G \equiv G_{ii}$, $F \equiv F_{ii}$, and $\Delta \equiv \Delta_{ii}$ is introduced for the diagonals and $\tilde{G} \equiv G_{ij}$, $\tilde{F} \equiv F_{ij}$, and $\tilde{\Delta} \equiv \Delta_{ij}$ for the nondiagonal ($i \neq j$) Green's function and order parameters. The determinant of the system of Eq. (11) for real Δ and $\tilde{\Delta}$ has the form

$$D(\omega) = [\omega^2 - \omega_+^2(\xi)][\omega^2 - \omega_-^2(\xi)], \tag{12}$$

where

$$\begin{aligned} \omega_+(\xi) &= \sqrt{\xi^2(\mathrm{p}) + [\Delta + (l-1)\tilde{\Delta}]^2}, \\ \omega_-(\xi) &= \sqrt{\xi^2(\mathrm{p}) + (\Delta - \tilde{\Delta})^2}. \end{aligned} \tag{13}$$

It follows from this that the quasiparticle spectrum in the SC state with several ($l \geqslant 2$) equivalent valleys (FS packets) is characterized for $T \to 0$ by two gaps

$$\Delta_+ = \Delta + (l-1)\tilde{\Delta}, \quad \Delta_- = |\Delta - \tilde{\Delta}|, \tag{14}$$

and the order parameters Δ and $\tilde{\Delta}$ in the weak-binding approximation are determined by the integral equations

$$\begin{aligned} \Delta = \frac{1}{(2\pi)^4} \int d\mathrm{p} d\omega \{ & [V + (l-1)U] F(\mathrm{p}, \omega) \\ & + (l-1)[2W + (l-2)U] \tilde{F}(\mathrm{p}, \omega)\}, \end{aligned} \tag{15}$$

$$\begin{aligned} \tilde{\Delta} = \frac{1}{(2\pi)^4} \int d\mathrm{p} d\omega \{ & [\tilde{V} + (l-1)U + 2(l-2)W \\ & + (l-2)^2 U] \tilde{F}(\mathrm{p}, \omega) + [2W + (l-2)U] F(\mathrm{p}, \omega)\}, \end{aligned} \tag{16}$$

where

$$\begin{aligned} & V \equiv W_{ii,ii}, \quad \tilde{V} \equiv W_{ij,ij} = W_{ji,ji}, \\ & W \equiv W_{ii,ij} = W_{ii,ji} = W_{ij,ii} = W_{ji,ii}, \\ & U \equiv W_{ii,jj} = W_{jj,ii} = W_{ij,ji} = W_{ji,ij}. \end{aligned} \tag{17}$$

For $T \to T_c$ the linearized system of equations (15) and (16) gives rise to the form

$$\begin{aligned} & \Delta\left(1 - \lambda_l \ln \frac{\bar{\omega}_{ph}}{T_c}\right) - (l-1)\rho_l \tilde{\Delta} \ln \frac{\bar{\omega}_{ph}}{T_c} = 0, \\ & -\rho_l \Delta \ln \frac{\bar{\omega}_{ph}}{T_c} + \tilde{\Delta}\left\{1 - \left[\tilde{\lambda}_l + (l-2)\rho_l \ln \frac{\bar{\omega}_{ph}}{T_c}\right]\right\} = 0, \end{aligned} \tag{18}$$

where

$$\begin{aligned} & \lambda_l = -N(0)[V + (l-1)U], \quad \tilde{\lambda}_l = -N(0)[\tilde{V} + (l-1)U], \\ & \rho_l = -N(0)[2W + (l-2)U]. \end{aligned} \tag{19}$$

Under the conditions $V = \tilde{V}$ and $\lambda_l = \tilde{\lambda}_l$ we obtain from Eq. (17) [see Eq. (9)]

$$T_c \approx \bar{\omega}_{ph} \max\{\exp(-1/\Lambda_\pm)\}, \tag{20}$$

where

$$\Lambda_+ \equiv \lambda_l - \rho_l, \quad \Lambda_- \equiv \lambda_l + (l-1)\rho_l. \tag{21}$$

It can be seen that independently of the sign of the constant ρ_l the intervalley interaction promotes an increase in T_c. Thus for $\rho_l > 0$ the constant λ in Eq. (10a), according to Eqs. (19) and (21), should be replaced by the quantity

$$\Lambda_- = \lambda + (l-1)[\tilde{\varkappa} + (l-1)\tilde{\tilde{\varkappa}}], \tag{22}$$

where

$$\lambda \equiv -N(0)V, \quad \tilde{\varkappa} \equiv -2N(0)W, \quad \tilde{\tilde{\varkappa}} \equiv -N(0)U, \tag{23}$$

while $l = 8$ according to the number of equivalent degenerate valleys at L-points of the BZ. If the main contribution to the DS of the state of A_3C_{60} comes from deeper nondegenerate valleys at the X-points of the BZ, then $l = 6$ (see Ref. 30) and the effective coupling constant [Eq. (10a)] is $\lambda = \lambda_1$.

4. CONCLUSIONS

The dynamic Jahn–Teller effect and the multivalley electron spectrum associated with the high symmetry of C_{60} molecules and A_3C_{60} can thus be the reason for HTSC in doped fullerite, due to the enhancement of the EPI [see Eqs. (10) and (22)].

We note that for $x \neq 3$ the disorder introduced by doping leads to mixing of the states from different valleys (this occurs for the condition $\tau_{ij}\tilde{\Delta} \ll 1$, i.e., in the limiting case of a "dirty" superconductor[40]) and this reduces the efficiency of the intervalley interaction mechanism. The sharp maximum in T_c at the stoichiometric composition ($x = 3$) of doped fullerites A_xC_{60} can evidently be explained in this way.

On the other hand, crystals consisting of C_{70} molecules are anisotropic and, consequently, the number of equivalent degenerate valleys in them should be fewer than in the BZ of isotropic cubic crystals of the fullerite C_{60}. In addition, as noted above, in C_n molecules with $n \geqslant 70$ the Jahn–Teller effect can be absent from the actual electron terms. In this connection it is most probable that in A_xC_{70} the FL arising in the process of doping intersects only one nondegenerate band with a small number of valleys (2–4) so that (other conditions being equal) for systems containing C_{70} the values of T_c should be much lower than in systems based on C_{60}, or the SC transition might be completely absent.

In conclusion we note that in the cubic perovskite $BaBiO_3$, doped with potassium,[12] T_c may also be raised by the Jahn–Teller pseudoeffect in the symmetric oxygen octahedra, since in layered copper metal oxides with a damaged perovskite symmetry the nature of the HTSC could be different (see, for example, Ref. 41); however, this does not exclude an important role for the EPI.

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[1] We note that for the stoichiometric composition in the compound A_3C_{60} (or ATl_2C_{60}), when the alloying atoms (donors) fill the whole free intersite space, the symmetry of the lattice and of the BZ is not destroyed.

[2] It might be thought that with the dynamical mechanism for lifting the degeneracy of the bands, coherent interband Cooper pairing would not have time to occur, which distinguishes this model from the standard model of a two-band metal[35,36] in which only interband pairing is taken into account.

[3] The last inequality indicates that intravalley electron scattering by defects and impurities leads to rapid production of momentum isotropy of their spectrum, i.e., the FS in each valley can be considered spherical.

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