Alexandrov and Bratkovsky Reply: In our Letter [1] we proposed a theory of ferromagnetism and colossal magnetoresistance (CMR) based on the idea of a current carrier density collapse due to pairing of polaronic carriers in doped ferromagnetic semiconductors. Nagaev [2] has neglected the fact that the theory is largely independent of the type of electron-phonon interaction and of a particular orbital state of holes.

Nevertheless, the Comment raises a key question about the essential interactions in oxides. Here we show that the radical claims [2,3] that (i) small polarons do not exist in manganites and (ii) there is no convincing proof that they exist in *any* other semiconducting materials are wrong. The problem stems from an incorrect estimate of the polaron binding energy  $E_{\rm SP}$  (polaron shift) in [2,3]. Instead, one should use the exact expression for  $E_{\rm SP}$  (see, e.g., Ref. [4]) with the *experimental* dielectric constants. For the Fröhlich interaction,

$$E_{\rm SP} = \frac{1}{2\kappa} \int_{\rm BZ} \frac{d^3 q}{(2\pi)^3} \frac{4\pi e^2}{q^2} \,, \tag{1}$$

where the dielectric constants,  $\kappa^{-1} = \epsilon_{\infty}^{-1} - \epsilon_{0}^{-1}$ , are known from experiment, and the size of the integration region [the Brillouin zone (BZ)] is determined by the lattice constants a, b, c (Table I). Nagaev's formula for  $E_{\rm SP}$  is numerically wrong because of an inaccurate lower limit in the integral (which underestimates  $E_{\rm SP}$  by a factor of 2) and inaccurate data for the dielectric constants.

The actual value for  $E_{\rm SP}$  is of the order of 1 eV (Table I), much larger than Nagaev's estimate,  $\sim 0.15$  eV. Note that the data in the table represent the *lower* boundary for the  $E_{\rm SP}$ , since the long-wave approximation for the matrix element, Eq. (1), underestimates the contribution of the short-wave optical phonons. Also, short-wave acoustic

TABLE I. Polaron shift  $E_{\rm SP}$  due to Fröhlich interaction. The data are from Ref. [9]. The value  $\epsilon_{\infty}=5$  for WO<sub>3</sub> is an estimate.

			$a \times b \times c$	$E_{SP}$
System	$oldsymbol{\epsilon}_{\infty}$	$\epsilon_0$	(Å)	(eV)
$BaTiO_3$	5.1 - 5.3	1499	$3.992^2 \times 4.032$	0.842
La <sub>2</sub> CuO <sub>4</sub>	5.0	30	$3.8^{2} \times 6^{a}$	0.647
$LaMnO_3$	3.9 <sup>b</sup>	16 <sup>b</sup>	$3.86^{3}$	0.884
$La_{2-2x}Sr_{1+2x}$			•••	
$-Mn_2O_7$	4.9 <sup>b</sup>	38 <sup>b</sup>	$3.86^2 \times 3.9^a$	0.807
$SrTiO_3$	5.2	310	$3.905^3$	0.852
$WO_3$	5	100 - 300	$7.31 \times 7.54 \times 7.7$	0.445
CdO	5.4	21.9	$4.7^{3}$	0.522
EuS	5.0	11.1	$5.968^{3}$	0.324
EuSe	5.0	9.4	$6.1936^3$	0.266
MgO	2.964	9.816	$4.2147^3$	0.982
NaCl	2.44	5.90	$5.643^3$	0.749
NiO	5.4	12	$4.18^{3}$	0.429
$TiO_2$	6 - 7.2	89 - 173	$4.59^2 \times 2.96$	0.643

<sup>&</sup>lt;sup>a</sup>Distance between CuO<sub>2</sub> or MnO<sub>2</sub> planes. <sup>b</sup>Reference [10].

and/or Jahn-Teller phonons are not included. The large value of the polaron shift is compatible with the small-polaron theory [5].

Irrespective of any theoretical arguments, the existence of polarons in CMR materials is unambiguously confirmed experimentally, including very low mobility, activated dc and ac transport in the paramagnetic phase, and the giant isotope effect (for references, see [1]). Contrary to Nagaev's claim, the theory [1] well describes the optical properties of manganites, in particular the giant spectral weight transfer with temperature and magnetic field [6].

We conclude that all of the objections [2] against the (bi)polaron theory of CMR originate from complete disregard of abundant experimental data and a wrong estimate of the polaron binding energy. The theory suggests that by replacing the magnetic ions (Mn) with nonmagnetic ions (Cu), one can transform a doped charge-transfer insulator into a high-temperature superconductor owing to the Bose-Einstein condensation of bipolarons [4], as was observed experimentally [7]. Theories of CMR and/or high-temperature superconductivity based on the double-exchange interaction, and/or magnetic fluctuations alone do not take into account the *much stronger* Fröhlich interaction (Table I) [8].

We thank D. M. Eagles, T. Ishikawa, J. H. Jung, P. E. Kornilovitch, T. W. Noh, Y. Tokura, and G. M. Zhao for their data and discussions.

A. S. Alexandrov<sup>1</sup> and A. M. Bratkovsky<sup>2</sup>

<sup>1</sup>Department of Physics, Loughborough University Loughborough, LE11 3TU, United Kingdom <sup>2</sup>Hewlett-Packard Laboratories, 1501 Page Mill Ro

<sup>2</sup>Hewlett-Packard Laboratories, 1501 Page Mill Road Palo Alto, California 94304-1126

Received 18 May 1999

PACS numbers: 71.30.+h, 71.38.+i, 72.20.Jv, 75.50.Pp

- [1] A. S. Alexandrov and A. M. Bratkovsky, Phys. Rev. Lett. 82, 141 (1999).
- [2] E. L. Nagaev, preceding Comment, Phys. Rev. Lett. 84, 2042 (2000).
- [3] E. L. Nagaev, Phys. Lett. A 258, 65 (1999).
- [4] A. S. Alexandrov and N. F. Mott, *Polarons and Bipolarons* (World Scientific, Singapore, 1995).
- [5] For the Fröhlich interaction the small-polaron theory is numerically accurate even in the weak coupling regime. A. S. Alexandrov and P. E. Kornilovitch, Phys. Rev. Lett. **82**, 807 (1999).
- [6] A. S. Alexandrov and A. M. Bratkovsky, Phys. Rev. B 60, 6215 (1999); J. Phys. Condens. Matter 11, L531 (1999).
- [7] J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).
- [8] The Fröhlich interaction with high-frequency phonons cannot be screened by heavy polarons.
- [9] Handbook of Optical Constants of Solids, edited by E. D. Palik (Academic, New York, 1997); Landolt-Börnstein, New Series (Springer, Berlin, 1994).
- [10] T. Ishikawa (private communication).