

Comment on "Geometric Phase in Jahn-Teller Crystals"

In a recent Letter [1] Koizumi examines a Jahn-Teller solid. The starting point Hamiltonian is $H = \sum_j H_j + H_{\text{inter}}$. H_j describes a Jahn-Teller ion and reads

$$H_j = k\rho_j(e^{i\Theta_j}a_j^\dagger b_j + e^{-i\Theta_j}b_j^\dagger a_j) - \frac{1}{2}\rho_j^{-1/2}\frac{\partial^2}{\partial\rho_j^2}\rho_j^{1/2} + \frac{1}{8\rho_j^2} - \frac{1}{2\rho_j^2}\frac{\partial^2}{\partial\Theta_j^2} + \frac{1}{2}\rho_j^2. \quad (1)$$

a_j^\dagger, b_j^\dagger are fermion creation operators on the E orbitals of ion j . H_{inter} is a coupling between the phonon variables (ρ_j, Θ_j) at different sites which is specified in the continuum limit as a gradient term $(|\nabla_{\mathbf{x}}\phi|^2)$ with \mathbf{x} the continuum analog of i, j . The corresponding lattice version (not provided by Koizumi) would be

$$H_{\text{inter}} = \beta \sum_{\langle ij \rangle} |\phi_i - \phi_j|^2, \quad (2)$$

where β is a constant.

The author diagonalizes the electronic part to get the adiabatic electronic ground state in each ion,

$$|\psi_j^-\rangle = (1/\sqrt{2})e^{i\chi(\Theta_j)}(a_j^\dagger - e^{-i\Theta_j}b_j^\dagger)|0\rangle, \quad (3)$$

where $\chi(\Theta_j) = m_j\Theta_j$ with m_j an integer (or in the continuum and in the notation of Ref. [1] $\gamma = m\xi$). Usually one would put $m_j = 0$, but the author claims that due to H_{inter} the total energy can depend on m_j . Next the author derives the Lagrangian density in the continuum limit and obtains the Meissner effect and flux quantization in two spatial dimensions. Our claim is that these results are wrong because of the following reasons.

(1) The Hamiltonian commutes with the local number operator $n_j = a_j^\dagger a_j + b_j^\dagger b_j$ so local charges are conserved and the system is an insulator [2].

The current density operator is given in Eq. (21) of Ref. [1] where the field operators can be expanded in terms of a single particle basis set, $\psi(\mathbf{r}) = \sum_i \phi_i^a(\mathbf{r})a_i + \phi_i^b(\mathbf{r})b_i$. Here $\phi_i^a(\mathbf{r}), \phi_i^b(\mathbf{r})$ are Wannier functions corresponding to the two atomic orbitals in atom i . The gradient here is understood to be with respect to the \mathbf{r} coordinate [3] and not with respect to the continuous analog of the i index as was erroneously done in Ref. [1]. It is easy to check that the terms in the current operator that involve different atoms vanish due to the conservation of the local charges so a macroscopic Meissner current is not possible.

(2) The Hamiltonian for the vibrational motion of the Jahn-Teller solid on the lower potential surface has the kinetic term $-\sum_j \frac{1}{2}(1/\rho_j^2)[(\partial/\partial\Theta_j) + m_j - \frac{1}{2}]^2$ [Eqs. (3) and (4) of Ref. [1]]. The m_j can be trivially eliminated by the gauge transformation $\Psi \rightarrow \Psi e^{-i\sum_j m_j\Theta_j}$ so the m_j

have no physical consequences as it should be. H_{inter} is of no consequence for this conclusion which, of course, holds also for a single ion. The $\frac{1}{2}$ which originates in the legitimate Berry's phase cannot be eliminated (see below).

(3) The correct Lagrangian density in the continuum can be easily derived from the Lagrangian version of Eqs. (3)–(6) of Ref. [1] corresponding to a single ion [4]:

$$L_j = \frac{1}{2}|\dot{\phi}_j|^2 + \frac{1}{2}(\dot{\phi}_j\alpha_j^* + \dot{\phi}_j^*\alpha_j) - \frac{1}{2}|\phi_j|^2 + k|\phi_j| - \frac{1}{8|\phi_j|^2}$$

with $\alpha_j = -i(m_j - 1/2)e^{i\Theta_j}/\rho_j$, and is given by

$$\mathcal{L} = \frac{\sigma}{2}|\dot{\phi}|^2 + \frac{\sigma}{2}(\dot{\phi}\alpha^* + \dot{\phi}^*\alpha) - \frac{B}{2}|\nabla_{\mathbf{x}}\phi|^2 - \frac{A}{2}|\phi|^2 + C|\phi| - \frac{D}{|\phi|^2}. \quad (4)$$

$\sigma, A, B, C,$ and D are constants.

The form of the gauge fields bears no resemblance with the form given in Eq. (10) of Ref. [1]. Koizumi obtains this equation by averaging a phonon Lagrangian on the electronic adiabatic ground state. This is incorrect because the Lagrangian he starts with is already averaged and has no electronic coordinates.

The Lagrangian Eq. (4) has ordinary equations of motion and does not show the exotic effects claimed in Ref. [1]. In fact, the term with the gauge field can be rewritten as $\frac{1}{2}(\dot{\phi}\alpha^* + \dot{\phi}^*\alpha) = -(m - 1/2)\dot{\Theta}$ which is a total time derivative and can be eliminated from the Lagrangian either in the continuum or for the single ion in a classical computation.

It is interesting to remark that also the $\frac{1}{2}$, the legitimate Berry's phase disappears in the Lagrangian whereas it subsists in the Hamiltonian. This is because the gauge field produces a magnetic field which is zero everywhere except at the origin and is of no consequence at the classical level. This implies that Berry's phase has no effect in the collective motion of the lattice (there is no renormalization of the Goldstone mode) and neither in the classical motion of the slow variables of the single ion.

J. Lorenzana

CONICET, Centro Atómico Bariloche
8400 S.C. de Bariloche, Argentina

Received 3 February 1997 [S0031-9007(98)06557-0]
PACS numbers: 71.38.+i, 63.10.+a, 71.10.Hf, 82.90.+j

- [1] H. Koizumi, Phys. Rev. Lett. **76**, 2370 (1996).
- [2] This and the following conclusions do not depend on whether H_{inter} is taken in the continuous or in the lattice version.
- [3] G. D. Mahan, *Many-Particle Physics* (Plenum Press, New York, 1990), p. 30.
- [4] R. Jackiw, Comments At. Mol. Phys. **21**, 71 (1988).