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LETTER TO THE EDITOR

Decoupling of charge and spin density waves for a one-dimensional electron–phonon Peierls system with a half-filled band

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Abstract. Decoupling of charge and spin density waves for a Peierls electron-phonon system with a half-filled band (polyacetylene) was achieved as a consequence of the vanishing of certain interaction terms in the fermion representation of electron field operators including spins due to the Pauli principle.

The off-diagonal electron-phonon coupling in a one-dimensional electron-phonon (Peierls) chain with half-filled band (trans-polyacetylene) results in the coupling of charge and spin density waves in the continuous limit in the respective boson representation (e.g. Hara and Fukuyama 1983). The separation of charge and spin solitons has been performed exactly only for a special choice of the Coulomb interactions, or numerically for more general cases.

In this letter we shall show that, besides other terms, terms like $(\psi^+_{1\sigma}(x)\psi_{2\sigma}(y))^2$ also appear in the Hamiltonian of electron–electron interactions mediated by phonons which vanish identically due to the Pauli principle. Using this already in the fermion representation of the electron field operator with spin an essential simplification of the interaction term is performed. As a result, we achieved the decoupling of charge and spin density waves in the respective boson representation. However, although both waves are decoupled, both of them are substantially present, i.e. coexistent in the case with spin.

On the other hand, contributions of umklapp terms $\psi^+_{1\sigma}(x)\psi_{2\sigma}(y)\psi^+_{1\sigma'}(y)\psi_{2\sigma'}(x)$, $\sigma \neq \sigma'$, do not vanish even in the local limit $x = y$ in the present case. In the spinless case, however, the contribution of quantum fluctuations which result from umklapp terms in a more rigorous limit $y = x + a$ (a being the lattice constant) is relevant (Fradkin and Hirsch 1983). Hence, we can use the local limit $x = y$ in the present (spin) case.

Since the essential step of our derivation occurs during intermediate calculations when proceeding to the boson representation we summarise briefly the formalism necessary for the derivation of the respective form of the electron–electron interaction mediated by phonons.

Let the one-dimensional electron-phonon chain be defined by the Su-Schrieffer-Heeger (1979) Hamiltonian

$$H_{\mathrm{SSH}} = \sum_j \tfrac{1}{2}M\dot{q}_j'^2 + \tfrac{1}{2}D(q_j - q_{j+1})^2 - \sum_{j,\sigma}[t + \alpha(q_j - q_{j+1})](a^+_{j,\sigma}a_{j+1,\sigma} + \mathrm{HC}) \tag{1}$$

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with

$$u_j = -\frac{\alpha}{D}\sum_\sigma (a^+_{j,\sigma}(t)a_{j+1,\sigma}(t) + \text{HC}) \qquad u_j = q_{j+1} - q_j \tag{2}$$

as a solution to the dynamic equation for the phonon coordinate when the proper phonon dynamics is not accounted for. The Hamiltonian of the electron-electron interaction mediated by phonons is then

$$H^{(\text{ph})}_{\text{e-e}} = -g^2 \sum_j \left(\sum_\sigma a^+_{j,\sigma}a_{j+1,\sigma} + \text{HC}\right)^2 \qquad g^2 = \alpha^2/2D. \tag{3}$$

The transition to a continuous representation for the case of dimerisation $2k_F a = \pi$ (e.g. trans-polyacetylene) is realised by (Emery 1979)

$$\begin{aligned} a_{2n,\sigma}(t) &\to i^{2n}(2a)^{1/2}\psi_{E,\sigma}(x, t) \\ a_{2n+1,\sigma}(t) &\to i^{2n+1}(2a)^{1/2}\psi_{0,\sigma}(y, t) \end{aligned} \tag{4}$$

where $n \to \infty$ as $a \to 0$ in such a way that $2na \to x$ and $(2n+1)a \to y$.

In the representation which diagonalises the free part of the Hamiltonian

$$\psi_{1\sigma} = \frac{1}{\sqrt{2}}(\psi_{E,\sigma} + \psi_{0,\sigma}) \qquad \psi_{2\sigma} = \frac{1}{\sqrt{2}}(\psi_{E,\sigma} - \psi_{0,\sigma}) \tag{5}$$

the interaction Hamiltonian (3) becomes

$$-\tfrac{1}{4}g^2a^2 \lim_{y\to x}\left(\sum_\sigma \psi^+_{1\sigma}(x)\psi_{2\sigma}(y) + \psi^+_{1\sigma}(y)\psi_{2\sigma}(x) - \psi^+_{2\sigma}(y)\psi_{1\sigma}(x) - \psi^+_{2\sigma}(x)\psi_{1\sigma}(y)\right)^2. \tag{6}$$

With the use of boson representation ϕ of the fermion operators ψ (Luther and Peschel 1974, Emery 1979) it transforms to

$$\left(\sum_\sigma (\psi^+_{1\sigma}(x)\psi_{2\sigma}(x) - \psi^+_{2\sigma}(x)\psi_{1\sigma}(x))\right)^2$$

$$= \frac{4}{\pi^2a^2}\cos^2((2\pi)^{1/2}\phi_c)\cos^2((2\pi)^{1/2}\phi_s) \tag{7}$$

which recovers the result by Hara and Fukuyama. Here ϕ_c and ϕ_s are boson operators for charge and spin density waves. However, the left-hand side of (7) can be rewritten as

$$\sum_\sigma (\psi^+_{1\sigma}\psi_{2\sigma} - \psi^+_{2\sigma}\psi_{1\sigma})^2 + \frac{1}{\pi^2a^2}[\cos(8\pi)^{1/2}\phi_c) + \cos((8\pi)^{1/2}\phi_s)]. \tag{8}$$

The coupling is contained in the first term on the right-hand side which, in the terms of the boson fields, becomes

$$\sum_\sigma (\psi^+_{1\sigma}(x)\psi_{2\sigma}(x) - \psi^+_{2\sigma}(x)\psi_{1\sigma}(x))^2$$

$$= \frac{1}{\pi^2a^2}[1 + \cos((8\pi)^{1/2}\phi_c)\cos((8\pi)^{1/2}\phi_s)]. \tag{9}$$

This expression, substituted into (8), leads to the expression (7). On the other hand, the left-hand side of the equation (9) can be alternatively expressed as

$$\sum_{\sigma}(2\rho_{1\sigma}\rho_{2\sigma}-\rho_{1\sigma}-\rho_{2\sigma}) \tag{10}$$

where $\rho_{i\sigma}=\psi^{+}_{i\sigma}\psi_{i\sigma}$, $i=1,2$.

The terms $(\psi^{+}_{1\sigma}(x)\psi_{2\sigma}(x))^2$, $(\psi^{+}_{2\sigma}(x)\psi_{1\sigma}(x))^2$ in equation (9) vanish due to the Pauli principle.

Finally, the interaction term can be rewritten as

$$\sum_{\sigma}\rho_{1\sigma}\rho_{2\sigma}=\rho_{1c}\rho_{2c}+\rho_{1s}\rho_{2s} \tag{11}$$

i.e. the charge and spin density waves become decoupled. Decoupling of the components $l=1,2$ is easy to perform by a suitable Bogoliubov transformation. Further, we can simply add Coulomb interactions (Sólyom 1979) so that we have

$$H=v_{F_c}\int \mathrm{d}x\,\tfrac{1}{2}(\partial_\mu\phi_c)^2-\frac{v_F}{\pi a^2}(\gamma_{3\perp}+2\Gamma^2)\int \mathrm{d}x\cos((8\pi)^{1/2}\,\mathrm{e}^{\varphi_c}\phi_c)+v_{F_s}\int \mathrm{d}x\,\tfrac{1}{2}(\partial_\mu\phi_s)^2$$
$$+\frac{v_F}{\pi a^2}(\gamma_{1\perp}-2\Gamma^2)\int \mathrm{d}x\cos((8\pi)^{1/2}\,\mathrm{e}^{\varphi_s}\phi_s) \tag{12}$$

where

$$\begin{aligned} v_{F_c}&=v_F[(1+\gamma_{4\perp})^2-(\gamma_{2\parallel}+\gamma_{2\perp}-\gamma_{1\parallel}+4\Gamma^2)^2]^{1/2}\equiv v_F Q_c\\ v_{F_s}&=v_F[(1-\gamma_{4\perp})^2-(\gamma_{2\parallel}-\gamma_{2\perp}-\gamma_{1\parallel}+4\Gamma^2)^2]^{1/2}\equiv v_F Q_s \end{aligned} \tag{13}$$

and

$$\gamma_{i\alpha}=\frac{g_{i\alpha}a}{2\pi v_F}\qquad \Gamma^2=\frac{g^2 a}{2\pi v_F}$$

$g_{i\alpha}$ being the Coulomb interaction constants and φ_c and φ_s the respective angles of the Bogoliubov rotation.

Rescaling ϕ_c and ϕ_s as $\phi_c\to(Q_c)^{1/2}\phi_c$, $\phi_s\to(Q_s)^{1/2}\phi_s$ we get finally the normal form of the Hamiltonian:

$$H=v_F\Big\{\int \mathrm{d}x\,\tfrac{1}{2}(\partial_\mu\phi_c)^2-\frac{1}{\pi a^2}(\gamma_{3\perp}+2\Gamma^2)\int \mathrm{d}x\cos(\beta_c\phi_c)+\int \mathrm{d}x\,\tfrac{1}{2}(\partial_\mu\phi_s)^2$$
$$+\frac{1}{\pi a^2}(\gamma_{1\perp}-2\Gamma^2)\int \mathrm{d}x\cos(\beta_s\phi_s)\Big\}. \tag{14}$$

Here

$$\begin{aligned} \beta_c^2&=\frac{8\pi}{Q_c}\,\mathrm{e}^{2\varphi_c}=\frac{8\pi}{1+\gamma_{4\perp}+\gamma_{2\parallel}+\gamma_{2\perp}-\gamma_{1\parallel}+4\Gamma^2}\\ \beta_s^2&=\frac{8\pi}{Q_s}\,\mathrm{e}^{2\varphi_s}=\frac{8\pi}{1-\gamma_{4\perp}+\gamma_{2\parallel}-\gamma_{2\perp}-\gamma_{1\parallel}+4\Gamma^2}. \end{aligned} \tag{15}$$

For completeness, let us remark that the resulting Hamiltonian (14) implies independent Kosterlitz–Thouless phase transitions to the dimerised charge and spin phases determined only by Coulomb interactions. The conditions for stability of charge and

spin density waves $\beta_c^2 < 8\pi$ and $\beta_s^2 < 8\pi$ (Coleman 1975) imply the respective phase transitions if

$$g_{c,\mathrm{crit}}^2 = \tfrac{1}{4}(g_{1\parallel} - g_{2\parallel} - g_{2\perp} - g_{4\perp}) > 0$$

$$g_{s,\mathrm{crit}}^2 = \tfrac{1}{4}(g_{1\parallel} - g_{2\parallel} + g_{2\perp} + g_{4\perp}) > 0.$$

If the Coulomb interactions were neglected then $g_{c,\mathrm{crit}} = g_{s,\mathrm{crit}} = 0$, i.e. we came to the conclusion obtained also by Fradkin and Hirsch that only the dimerised phases were stable.

Other mechanisms of coupling of spin and charge density waves are known (e.g. Sato 1983) which are not considered in the present paper.

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