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Thermodynamics of the SO(4) x SO(4)
submodel

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Dynamical SU(8) for phase-coexistence: Thermodynamics of the SO(4) $\times$ SO(4) submodel*

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Abstract

We review a scheme for describing a multi-phase interacting system of electrons within the dynamical algebra su(8): we discuss the thermodynamics of a submodel which incorporates the relevant physics, and has so(4) $\oplus$ so(4) for its dynamical algebra.

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We first write down a mean-field hamiltonian H in terms of electron annihilation (creation) operators $a_{k\sigma}(a^t_{k\sigma})$ which satisfy the anti-commutation relation:

$$\{a_{k\sigma}, a^t_{k'\sigma'}\} = \delta_{kk'}, \delta_{\sigma\sigma'}. \tag{1}$$

and which incorporates (apart from the kinetic energy term H_{KE}) singlet superconductivity (H_{SC}), charge-density (H_{CDW}) and spin-density wave (H_{SDW}) terms. Thus

$$H \quad = H_{KE} + H_{SC} + H_{CDW} + H_{SDW} \tag{2}$$

where

$$H_{KE} \quad = \Sigma\epsilon(k) a^\dagger_{k\sigma} a_{k\sigma} \tag{3}$$

$$H_{SC} \quad = \Sigma\Delta^* a_{k\uparrow} a_{-k\downarrow} + \text{h.c.} \tag{4}$$

$$H_{CDW} \quad = \Sigma\gamma_0 a^\dagger_{k+Q\sigma} a_{k\sigma} + \text{h.c.} \tag{5}$$

$$H_{SDW} \quad = \Sigma a^\dagger_{k+Q} \underline{\gamma} \cdot \underline{\sigma} a_k + \text{h.c.} \tag{6}$$

Here expressions 3–6 are standard, with $Q = 2k_F$ (k_F is the wave vector of the fermi level) a characteristic wave vector for density wave order. [Summation $\sum$ over repeated indices and over implied spin indices in (6).] With the additional simplification that there is no contribution from terms for which $|k| > Q$, we may write H as a direct sum, $H = \oplus_k^{k_F} H(k)$; $H(k)$ is a hermitian bilinear in $B_i(k)$, where (writing $\bar{k} = k - Q$)

$$\{B_i(k)\} = \{a_{k\uparrow}, a^\dagger_{-kl}, a_{\bar{k}\uparrow}, a^\dagger_{-\bar{k}\downarrow}; a_{k\downarrow}, a^\dagger_{-k\uparrow}, a_{\bar{k}\downarrow}, a^\dagger_{-\bar{k}\uparrow}\} \tag{7}$$

As in (1), $\{B_i, B_j^\dagger\} = \delta_{ij}$ and the bilinears $X_{ij} \equiv B_i^\dagger B_j$ generate the Lie algebra $gl(8)$; the hermitian combinations occurring in the hamiltonian — which in addition has zero trace — may be shown to generate the whole of su(8)[1]. A physical consequence of this mathematical property is that, among others, triplet superconductivity terms are generated [2].

This su(8) model incorporates the mean field hamiltonian necessary for a discussion of coexistence of any of these phases (superconducting or density wave). However, a more tractable model which nonetheless encapsulates the essential features may be obtained by choosing only specified components of the density wave terms in (5) and (6) (γ_0 purely imaginary, real Δ and $\underline{\gamma}$ with $\underline{\gamma}$ along the third axis and assuming the so called "nesting" condition, $\epsilon(k) + \epsilon(\bar{k}) = 0$). The resulting hamiltonian δH may be written as

$$H = \oplus_k H(k),$$

where

$$
\begin{aligned}
H(k) = \quad & \epsilon(a^\dagger_{k\uparrow}a_{k\uparrow} + a^\dagger_{-k\downarrow}a_{-k\downarrow} + a^\dagger_{k\downarrow}a_{k\downarrow} + a^\dagger_{-k\uparrow}a_{-k\uparrow}) \\
& -\epsilon(a^\dagger_{\bar{k}\uparrow}a_{\bar{k}\uparrow} + a^\dagger_{-\bar{k}\downarrow}a_{-\bar{k}\downarrow} + a^\dagger_{\bar{k}\downarrow}a_{\bar{k}\downarrow} + a^\dagger_{-\bar{k}\uparrow}a_{-\bar{k}\uparrow} \\
& -\Delta(a^\dagger_{k\uparrow}a^\dagger_{-k\downarrow} + a^\dagger_{\bar{k}\uparrow}a^\dagger_{-\bar{k}\downarrow} - a^\dagger_{k\downarrow}a^\dagger_{-k\uparrow} - a^\dagger_{\bar{k}\downarrow}a^\dagger_{-\bar{k}\uparrow}) + \text{h.c.} \\
& +\tfrac{1}{2}\gamma_3(a^\dagger_{k\uparrow}a_{\bar{k}\uparrow} + a_{-k\downarrow}a^\dagger_{-\bar{k}\downarrow} - a^\dagger_{k\downarrow}a_{\bar{k}\downarrow} - a_{-k\uparrow}a^\dagger_{-\bar{k}\uparrow}) + \text{h.c.} \\
& +\tfrac{1}{2}i\gamma_0(a^\dagger_{k\uparrow}a_{\bar{k}\uparrow} - a_{-k\downarrow}a^\dagger_{-\bar{k}\downarrow} + a^\dagger_{k\downarrow}a_{\bar{k}\downarrow} - a_{-k\uparrow}a^\dagger_{-\bar{k}\uparrow}) + \text{h.c.}
\end{aligned}
\tag{8}
$$

We define operators $\underline{L}^\alpha, \underline{K}^\alpha$ ($\alpha =\uparrow$ or $\downarrow$) as follows:

$$
\begin{aligned}
L^\uparrow_3 &= \frac{1}{2}(a^\dagger_{k\uparrow}a_{k\uparrow} + a^\dagger_{-k\downarrow}a_{-k\downarrow} - a^\dagger_{\bar{k}\uparrow}a_{\bar{k}\uparrow} - a^\dagger_{-\bar{k}\downarrow}a_{-\bar{k}\downarrow}) \\
L^\uparrow_1 &= \frac{1}{2}(a^\dagger_{k\uparrow}a^\dagger_{-k\downarrow} + a^\dagger_{\bar{k}\uparrow}a^\dagger_{-\bar{k}\downarrow}) + \text{h.c.} \\
K^\uparrow_1 &= \frac{1}{2}(a^\dagger_{k\uparrow}a_{\bar{k}\uparrow} + a_{-k\downarrow}a^\dagger_{-\bar{k}\downarrow}) + \text{h.c.} \\
K^\uparrow_2 &= -\frac{i}{2}(a^\dagger_{k\uparrow}a_{\bar{k}\uparrow} - a_{-k\downarrow}a^\dagger_{-\bar{k}\downarrow}) + \text{h.c.}
\end{aligned}
$$

with similar expressions for $\underline{L}^\downarrow, \underline{K}^\downarrow$ with the spins reversed. Then $H(k)$ takes the form

$$H(k) = H^\uparrow(k) + H^\downarrow(k)$$

where

$$H^\alpha(k) = \underline{\lambda}^\alpha \cdot \underline{L}^\alpha + \underline{\kappa}^\alpha, \underline{k}^\alpha, \quad (\alpha =\uparrow \text{ or } \downarrow)$$

with

$$
\begin{aligned}
\underline{\lambda}^\uparrow &= (-2\Delta, 0, 2\epsilon); \underline{\kappa}^\uparrow = (\gamma_3, -\gamma_0, 0); \\
\underline{\lambda}^\downarrow &= (2\Delta, 0, 2\epsilon); \underline{\kappa}^\downarrow = (-\gamma_3, -\gamma_0, 0).
\end{aligned}
$$

Introducing operators $L^\uparrow_2, K^\uparrow_3$ as

$$
\begin{aligned}
L^\uparrow_2 &= -\frac{i}{2}(a^\dagger_{k\uparrow}a^\dagger_{-k\downarrow} - a^\dagger_{\bar{k}\uparrow}a^\dagger_{-\bar{k}\downarrow}) + \text{h.c.} \\
K^\uparrow_3 &= \frac{1}{2}(a^\dagger_{k\uparrow}a^\dagger_{-\bar{k}\downarrow} - a_{-k\downarrow}a_{\bar{k}\uparrow}) + \text{h.c.}
\end{aligned}
$$

and analogous expressions for $L^\downarrow_2, K^\downarrow_3$, the system of operators $\underline{L}^\alpha, \underline{K}^\alpha$ closes under the cummutation relations of so(4) $\oplus$ so(4):

$$
\begin{aligned}
&[L^\alpha_\ell, L^\beta_m] = i\delta^{\alpha\beta}e_{\ell mn}L^\alpha_n \\
&[L^\alpha_\ell, K^\beta_m] = i\delta^{\alpha\beta}e_{\ell mn}K^\alpha_n \\
&[K^\alpha_\ell, K^\beta_m] = i\delta^{\alpha\beta}e_{\ell mn}L^\alpha_n \qquad \ell, m, n = 1, 2, 3
\end{aligned}
$$

It follows immediately, on use of the two invariants $\lambda^2 + \kappa^2$ and $\underline{\lambda} \cdot \underline{\kappa}$ associated with SO(4), that the energy spectrum of the system has the values

$$E^{\pm}(k) = \frac{1}{2}[4\epsilon(k)^2 + \gamma_0^2 + (2\Delta \mp \gamma_3)^2]^{\frac{1}{2}}. \tag{9}$$

The hamiltonian $H(k)$ may be rotated to a sum of the Cartan elements of the algebra (L_3^α, K_3^α) by the rotation $R(k)$,

$$R(k) = e^{i\phi_2(L_2^\uparrow - L_2^\downarrow)} e^{i\phi_2'(K_2^\uparrow - K_2^\downarrow)} e^{i\phi_1(K_1^\uparrow + K_1^\downarrow)} \tag{10}$$

with

$$\begin{aligned} \phi_1 &= \tan^{-1}(\gamma_0/2\epsilon) \\ \phi_2 &= -(1/2)\tan^{-1}\{4\Delta(4\epsilon^2 + \gamma_0^2)^{\frac{1}{2}}/(4\epsilon^2 + \gamma_0^2 + \gamma_3^2 - 4\Delta^2)\} \\ \phi_2' &= (1/2)\tan^{-1}\{2\gamma_3(4\epsilon^2 + \gamma_0^2)^{\frac{1}{2}}/(4\epsilon^2 + \gamma_0^2 - \gamma_3^2 + 4\Delta^2)\} \end{aligned} \tag{11}$$

[The index k is suppressed in (12).]
In addition to this inner automorphism of so(4)$\oplus$so(4), a further rotation R_0, which is an element of SU(8) but an outer automorphism of so(4)$\oplus$so(4) is necessary in order to send the Cartans into a sum of number operators $M_i \equiv B_i^\dagger B_i$, thus diagonal in Fock space. (In the basis (4) R_0 may be chosen to be $\exp \frac{i\pi}{4}(\tau_0 \times \tau_1 \times \tau_2)$.)

The ground state (temperature $\tau = 0$) properties of this model were discussed in reference [2]: we now proceed to a discussion of the thermodynamics.

The thermodynamics of the system $H = \oplus H(k)$ is particularly straightforward. Thus the partition function Z may be written

$$Z \equiv Tr\exp(-\beta H) = Tr\exp(-\beta \Sigma H(h)) = \prod_k Z(k) \qquad [\beta = (k_B T)^{-1}]$$

where $Z(k) = tr(\exp -\beta H(k))$ is the partition function restricted to the k-system. (Tr is the trace over all states, tr over the k-states only.) Similarly for an operator $Q = \sum_k Q(k)$, we may easily see that

$$\langle\langle Q \rangle\rangle_\beta \equiv Tr\exp(-\beta H)Q/Z = \sum_k \langle\langle Q(k) \rangle\rangle_\beta.$$

If under the diagonalizing rotation — valid even in the su(8) case —

$$H(k) \longrightarrow \sum_{i=1}^{8} E_i n_i$$

$$Q(k) \longrightarrow \sum_{i=1}^{8} \mu_i n_i + (\text{non-diagonal terms})$$

then one may evaluate readily

$$\langle\langle Q(k)\rangle\rangle_\beta = \sum_{i=1}^{8} \mu_i (e^{\beta E_i} + 1)^{-1}.$$

In the so(4)⊕so(4) case, we have

$$\{E_i\} = \{E^+, E^-, -E^+, -E^-; E^+, E^-, -E^+, -E^-\}$$

where $E^{\pm}$ are given in (11), similarly for the rotated $Q(k)$

$$\{\mu_i\} = \{\mu_+, \mu_-, -\mu_+, -\mu_-; \mu_+, \mu_-, -\mu_+, -\mu_-\}$$

so that in general we have

$$\langle\langle Q(k)\rangle\rangle_\beta = -2\mu_+ \tanh\frac{1}{2}\beta E^+ - 2\mu_- \tanh\frac{1}{2}\beta E^-$$

In the same way, the average total energy of the system may be written

$$\langle\langle H(k)\rangle\rangle_\beta = -2\{E^+ \tanh\frac{1}{2}\beta E^+ + E^- \tanh\frac{1}{2}\beta E^-\}.$$

Choosing the negative square root values in (10), we see that the zero-temperature limit ($\beta \to \infty$) is given by

$$\langle\langle H(k)\rangle\rangle_\infty = 2(E^+ + E^-).$$

This corresponds to a filled Fermi sea ground state. The analogous zero-temperature order parameters are

$$\langle\langle Q(k)\rangle\rangle_\infty = 2(\mu_+ + \mu_-).$$

All 12 operators in so(4)⊕so(4) may be identified with physical processes; six have zero-thermodynamic expectation at all temperatures. In the appended table we give the thermodynamic and ground state ($\beta = \infty$) expectations for the six non-vanishing operators; the latter values are in complete accord with the zero-temperatue calculations of reference [2].

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References

[1] A.I. Solomon and J.L. Birman, J.Math.Phys.28,1526(1987)

[2] A.I. Solomon and J.L. Birman, "Mechanism for Generation of triplet Superconductivity" [to be published].