An Effective Classical Field Hamiltonian for the Quantum $S = \frac{1}{2}$ Models.

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Field theories and renormalization group analyses have been proved very effective in studying the critical behaviour at phase transitions. In general quantum-mechanical effects are not considered in these theoretical approaches, because they are difficult to take into account and in several cases they may be negligible. On the other hand, pseudospin models have been proposed with quantum $S = \frac{1}{2}$ Hamiltonians for hydrogen-bonded crystals to describe the ferroelectric (1) order-disorder transitions and for lattice gas models of the Λ-transition in superfluid ^{4}He (2). Thus it might prove interesting to derive a field Hamiltonian for such models, in order to study their critical properties by the renormalization group approach. In this paper we show how it is possible to derive a classical Ising-type effective Hamiltonian for a $S = \frac{1}{2}$ quantum Hamiltonian of the form

$$H = H_0 + H' , \qquad H_0 = \sum_i H_{0i} , \qquad H' = \sum_{i,j}{}' H'_{ij} , \tag{1}$$

where H_{0i} is a one-spin Hamiltonian and H'_{ij} is a two-spin interaction (the primed summation symbol in (1) requires $i \neq j$). The derived Ising Hamiltonian is «effective» in the sense that it gives the same partition function for the system and consequently the correct thermodynamics. It can then be transformed into a field Hamiltonian by means of the standard Wilson's (3) procedure. The passage from the quantum-statistical mechanics problem to the corresponding classical one is exact in principle and it is made possible by the property that spin operators are traceless. In practice the results in noncommutative algebra available thus far (4) make the calculation possible only to the second-order in H' and one must require that

$$\|H_0\| \gg \|H'\| , \tag{2}$$

where $\|\cdot\|$ denotes the trace norm of the operators.

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(1) R. BLINC and S. SVETINA: *Phys. Rev.*, **147**, 423 (1966).
(2) P. R. ZILSEL: *Phys. Rev. Lett.*, **15**, 476 (1965); P. H. E. MEIJER and W. D. SCHERER: *Physica A (The Hague)*, **80**, 447 (1975).
(3) K. G. WILSON and J. KOGUT: *Phys. Rep. C*, **12**, 76 (1974).
(4) C. BUZANO, M. RASETTI and M. VADACCHINO: *J. Phys. A: Math. Nucl. Gen.*, **11**, 1001 (1978).

Notice that if one is interested in model Hamiltonians in which the dominant term is the two-spin interaction, just the mean field generalized procedure allows us to rewrite the Hamiltonian in the form of eq. (1), with the condition (2) satisfied in the small-fluctuation regime ([5]). We illustrate the proposed method for a model within this class: the Ising model in transverse field.

Let us consider more in detail the general Hamiltonian (1) (i, j run from 1 to N). All the operators in (1), as well as those to be considered in the following, belong to the vector space $\mathbf{\rho}$ over $\boldsymbol{C}$ generated by the ring $\mathbf{\Sigma} = \bigotimes_1^N \mathbf{\sigma}$ of the generalized Pauli matrices, $\mathbf{\sigma}$ being the ring of the Pauli matrices with the identity $\mathbf{\sigma} = \{\sigma^\alpha, I_2\}$, $\alpha = x, y, z$. In particular

$$\sigma_i^\alpha = I_2 \otimes I_2 \otimes \ldots \otimes \sigma_{i\text{-th}}^\alpha \otimes I_2 \otimes \ldots \otimes I_2 \,. \tag{3}$$

We consider also the sub-space $\mathbf{\rho}^z$ of $\mathbf{\rho}$ generated by the Abelian subring $\mathbf{\Sigma}^z = \bigotimes_1^N \mathbf{\sigma}^z$, where $\mathbf{\sigma}^z = \{\sigma^z, I_2\}$. The statistical mechanical problem is classical whenever $H \in \mathbf{\rho}^z$. It is to be emphasized that, as the trace of a direct product is the product of the traces, all elements of $\mathbf{\rho}$ are traceless except the multiples of the identity $\boldsymbol{I} \in \mathbf{\rho}$, where $\boldsymbol{I} = \bigotimes_1^N I_2$. A convenient basis for $\mathbf{\rho}$ is $\{\Gamma_{A_n}\}$, where

$$\Gamma_{A_n} = \sigma_{i_1}^{\alpha_1} \sigma_{i_2}^{\alpha_2} \ldots \sigma_{i_n}^{\alpha_n} \tag{4}$$

and $A_n = (i_1, i_2, \ldots, i_n; \alpha_1, \alpha_2, \ldots, \alpha_n)$ is a ordered multi-index ($i_1 < i_2 < \ldots < i_n$), n being the number of spin operators in the product on the r.h.s. of (4): obviously $\boldsymbol{I} = \Gamma_{A_0}$. The basis for the sub-space $\mathbf{\rho}^z$ is written as $\{\Gamma_{A_n^z}\}$, where $\Gamma_{A_n^z} = \sigma_{i_1}^z \sigma_{i_2}^z \ldots \sigma_{i_n}^z$. $\mathbf{\rho}$ is provided with a scalar product

$$(P, Q) = \frac{\mathrm{Tr}\{PQ\}}{\mathrm{Tr}\{\boldsymbol{I}\}}\,; \qquad P, Q \in \mathbf{\rho}\,. \tag{5}$$

Upon expanding P and Q by means of the basis, we obtain

$$(P, Q) = \sum_{A_n, B_m} P_{A_n} Q_{B_m} \frac{\mathrm{Tr}\{\Gamma_{A_n} \Gamma_{B_m}\}}{\mathrm{Tr}\{\boldsymbol{I}\}} = \sum_{A_n} P_{A_n} Q_{A_n}\,. \tag{6}$$

The identity (6) is true because $\Gamma_{A_n} = \Gamma_{A_n}^{-1}$, $\forall A_n$ and, as mentioned before, the multiples of $\boldsymbol{I}$ are the only elements of $\mathbf{\rho}$ not traceless. Equation (6) guarantees that (5) is indeed a scalar product. We have also that $P_{A_n} = (P, \Gamma_{A_n})$.

We use now the mathematical framework introduced above to compute the partition function for the Hamiltonian (1):

$$Z = \mathrm{Tr}\{\exp[-\beta H]\} = \mathrm{Tr}\{\exp[-\beta(H_0 + H')]\}\,. \tag{7}$$

As $H_0, H' \in \mathbf{\rho}$ do not commute with each other, we introduce the operator $V \in \mathbf{\rho}$ defined by

$$\exp[-\beta H] = \exp[-\beta H_0] \exp[-\beta V]\,, \tag{8}$$

([5]) *a*) C. Buzano, M. Rasetti and M. Vadacchino: *Lett. Nuovo Cimento*, **24**, 379 (1979); *b*) C. Buzano, M. Vadacchino and M. Rasetti: *Ferroelectrics*, **29**, 11 (1980).

V is evaluated by means of the inverse Backer-Campbell-Hausdorff formula recently derived up to second order in H' ([4]). Using (7), (8) and the definition (5), we can write the reduced partition function $Z' = 2^N Z$ (where $2^N = \mathrm{Tr}\{I\}$) as follows:

$$Z' = (\exp[-\beta H_0], \exp[-\beta V]) . \tag{9}$$

As H_0 is the sum of one-spin Hamiltonians we can choose a suitable local rotation:

$$\mathscr{R} = \bigotimes_1^N \mathscr{R}_i , \qquad \mathscr{R}_i = \exp[i\theta_i n_{i\alpha} \sigma^\alpha/2] , \tag{10}$$

such that $\tilde{H}_0 = \mathscr{R}^{-1} H_0 \mathscr{R} \in \rho^z$. Denoting by $\tilde{O} = \mathscr{R}^{-1} O \mathscr{R}$ the rotated operator corresponding to any $O \in \rho$, we can write

$$Z' = (\exp[-\beta \tilde{H}_0], \exp[-\beta \tilde{V}]) , \tag{11}$$

because $(\tilde{P}, \tilde{Q}) = (P, Q)$ due to the invariance of the traces under cyclic permutations. We notice in (11) that only the projection $\mathscr{P}_{\rho^z} \exp[-\beta \tilde{V}]$ onto ρ^z of $\exp[-\beta \tilde{V}]$ gives a nonzero contribution to Z' as $\exp[-\beta \tilde{H}_0] \in \rho^z$. We can then write

$$Z' = (\exp[-\beta \tilde{H}_0], \exp[-\beta V_{\mathrm{eff}}]) , \tag{12}$$

where

$$V_{\mathrm{eff}} = -\frac{1}{\beta} \ln \mathscr{P}_{\rho^z} \exp[-\beta \tilde{V}] \tag{13}$$

and the projector $\mathscr{P}_{\rho^z}$ acts simply as follows:

$$\mathscr{P}_{\rho^z} P = \sum_{A_n^z} (P, \Gamma_{A_n^z}) \Gamma_{A_n^z} = \sum_{A_n^z} P_{A_n^z} \Gamma_{A_n^z} . \tag{14}$$

Now, since $V_{\mathrm{eff}} \in \rho^z$, $\tilde{H}_0$ and V_{eff} commute and the partition function can be rewritten as

$$Z = \mathrm{Tr} \exp[-\beta H_{\mathrm{eff}}] , \tag{15}$$

where

$$H_{\mathrm{eff}} = \tilde{H}_0 + V_{\mathrm{eff}} . \tag{16}$$

$H_{\mathrm{eff}} \in \rho^z$ is now a classical Ising-type Hamiltonian: we remark as well that it is β-dependent through V_{eff}. Explicitly it has the general form

$$H_{\mathrm{eff}} = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{i_1, i_2, \ldots, i_n} \lambda^{(n)}_{i_1, i_2, \ldots, i_n} \sigma^z_{i_1} \sigma^z_{i_2} \ldots \sigma^z_{i_n} , \qquad i_k = 1 \ldots N . \tag{17}$$

For the Hamiltonian (17) one can use the Wilson's procedure to write a field Hamiltonian. In the general case this may be conplicated by nonlocal interactions (as eq. (17) shows), depending on the form of the original Hamiltonian.

As an exemplification, we outline the above procedure for the Ising model in transverse field, which is defined by the Hamiltonian

$$H = -\tfrac{1}{2}\sum_{i,j} J_{ij}\sigma_i^z\sigma_j^z - \Omega\sum_i \sigma_i^x - \sum_i h_i\sigma_i^z\,, \qquad J_{ii} = 0\,. \tag{18}$$

The Hamiltonian (18) can be rewritten in the form of eq. (1), with the condition (2) satisfied, by the generalized mean field procedure ([5,6]). Denoting by Π the spontaneous polarization:

$$\Pi = N^{-1}\langle\sum_i \sigma_i^z\rangle_{h_i=0}\,, \tag{19}$$

let us introduce the quantum fluctuations

$$\delta\sigma_i^z = \sigma_i^z - \Pi\,. \tag{20}$$

H' is then defined as the part of H bilinear in the $\delta\sigma_i^z$'s, namely

$$H' = -\tfrac{1}{2}\sum_{i,j} J_{ij}\,\delta\sigma_i^z\,\delta\sigma_j^z\,. \tag{21}$$

We obtain

$$H_{0i} = \tfrac{1}{2}N\Lambda\Pi^2 - N\Lambda\Pi\sigma_i^z - \Omega\sigma_i^x - h_i\sigma_i^z\,, \tag{22a}$$

$$H'_{ij} = -\tfrac{1}{2}J_{ij}\sigma_i^z\sigma_j^z + \Lambda\Pi(\sigma_i^z + \sigma_j^z) - \Lambda\Pi^2\,, \tag{22b}$$

where $\Lambda = N^{-1}\sum_k J_{k_0}$. The condition (2) is satisfied in the small-fluctuation regime $\|\delta\sigma_i^z\| \ll |\Pi|$.

The local rotation (10) is given by

$$\mathscr{R}_i = \exp\left[i\theta_i\sigma^y/2\right]; \qquad \theta_i = \operatorname{arctg}\left[\Omega/(N\Lambda\Pi + h_i)\right] \tag{23}$$

and for the rotated Hamiltonian $\tilde{H}_0 \in \boldsymbol{\rho}^z$ one has

$$\tilde{H}_0 = Nh_0 + \sum_i \Delta_i\sigma_i^z\,, \tag{24}$$

where $h_0 = \frac{1}{2}N\Lambda\Pi^2$ and $\Delta_i = \{\Omega^2 + (N\Lambda\Pi + h_i)^2\}^{\frac{1}{2}}$.

The operator V of the def. (8) can be written up to the second order in H' (notice; fourth order in the $\delta\sigma_i^z$'s). One has

$$V = V' + V'' + O(H'^3)\,, \tag{25a}$$

$$V' = \sum_{i,j} V'_{ij}\,, \qquad V'' = \sum_{i,j,m,l} V''_{ijml}\,, \tag{25b}$$

$$V'_{ij} = H'_{ij} + \sum_{n=1}^{\infty}\gamma^{(n)}\beta^n\boldsymbol{\sigma}_{ij}^{(n)}\,, \tag{25c}$$

$$V''_{ijml} = \sum_{n=2}^{\infty}\beta^n\left\{\sum_{k=1}^{n-1}\gamma_k^{(n)}\boldsymbol{\sigma}_n^{(k)}(ij/ml) + \frac{1}{2}\,\frac{(-)^n}{n!}\,\boldsymbol{\sigma}_n^{(n-1)}(ij/lm) + \right.$$
$$\left. + \frac{1}{2}\sum_{s=1}^{\infty}(-)^s\beta_{ij}^{n+s-1}\,\frac{1}{n!(n+s)!}\,[\boldsymbol{\sigma}_{ij}^{(n+s-1)}, \boldsymbol{\sigma}_{ml}^{(n-1)}]\right\}, \tag{25d}$$

([6]) C. BUZANO, M. RASETTI and M. VADACCHINO: *Prog. Theor. Phys.*, to be published.

where

$$\sigma_{ij}^{(n)} = \big[[\dots [H_0, \underbrace{H'_{ij}], \dots, H_0}_{n \text{ brackets}}], H_0\big], \tag{26a}$$

$$\sigma_n^{(k)}(ij/lm) = \Big[\Big[\Big[[\dots [H_0, \underbrace{H'_{ij}], H_0], \dots, H_0}_{k \text{ brackets}}], \underbrace{H'_{ml}\Big], H_0\Big], \dots, H_0}_{(n-k) \text{ brackets}}\Big], \tag{26b}$$

$\gamma^{(n)}$ and $\gamma_k^{(n)}$ are rational numbers given in ref. [5a].

Explicitly computing the operator $\tilde{V}$, one can check that, being $[I'_{A_n}, I_{A_1^z}] \perp \rho^z$, both $\rho_{ij}^{(n)} \perp \rho^z$, $\forall n, i, j$ and $\sigma_n^{(k)}(ij/ml) \perp \rho^z$, $\forall i, j, m, l, k < n-1$ (where $O \perp \rho^z$ is a shorthand notation to state $(O, P^z) = 0$, $\forall P^z \in \rho^z$). Computing V_{eff} up to the first order in H' (one must consistently expand up to the same order the ln and exp functions in eq. (13)), we obtain thus

$$V'_{\text{eff}} = \mathscr{P}_{\rho^z} \tilde{V}' = \mathscr{P}_{\rho^z} \tilde{H}' \tag{27}$$

and no true quantum-mechanical effect is retained, because eq. (27) is equivalent to consider H_0 and H' as commuting. The resulting effective Hamiltonian is simply

$$H'_{\text{eff}} = \tilde{H}_0 + \mathscr{P}_{\rho^z} \tilde{H}' = \sum_i (\Delta_i - N\Lambda\Pi\Psi_i)\sigma_i^z - \tfrac{1}{2}\sum_{i,j} J_{ij}\Psi_i\Psi_j\sigma_i^z\sigma_j^z\,, \quad \Psi_i = \sqrt{1-(\Omega/\Delta_i)^2}\,. \tag{28}$$

On the other hand, computing V_{eff} up to the second order in H', we write

$$V''_{\text{eff}} = \mathscr{P}_{\rho_z} \tilde{V}' + \mathscr{P}_{\rho^z} \tilde{V}'' + \frac{\beta}{2}[(\mathscr{P}_{\rho^z} \tilde{V}')^2 - \mathscr{P}_{\rho^z} \tilde{V}'^2]\,, \tag{29}$$

namely

$$H''_{\text{eff}} = H'_{\text{eff}} + \mathscr{P}_{\rho^z} \tilde{V}'' + \frac{\beta}{2}[(\mathscr{P}_{\rho^z} \tilde{V}')^2 - \mathscr{P}_{\rho^z} \tilde{V}'^2]\,. \tag{30}$$

We see that the second-order contribution to H_{eff} implies the calculation of $\sigma_{ij}^{(n)}$ together with their commutators as well as of $\sigma_n^{(n-1)}(ij/ml)$. However, the term quadrilinear in σ_i^z turns out to be zero and finally H''_{eff} reads

$$H''_{\text{eff}} = \sum_i \lambda_i^{(1)}\sigma_i^z + \frac{1}{2}\sum_{i,j} \lambda_{ij}^{(2)}\sigma_i^z\sigma_j^z + \frac{1}{3!}\lambda_{ijk}^{(3)}\sigma_i^z\sigma_j^z\sigma_k^z\,. \tag{31}$$

The coefficients $\lambda^{(n)}$ even though not so simple as for H'_{eff} yet can be now written explicitly. They involve rapidly convergent power series of the local fields Δ_i (indeed trascendental or generalized hypergeometrical functions). We do not write them at present: they will be reported in full detail elsewhere. The point we intend to comment about here is that now the Wilson's procedure can be applied. It leads, for a Hamiltonian of the form of H''_{eff} as given by (31), to a field Hamiltonian of the form

$$\mathscr{H} = \frac{1}{2}\{(\nabla\varphi)^2 + \mu^2\varphi^2\} + \frac{\lambda_3}{3!}\varphi^3 + \frac{\lambda_4}{4!}\varphi^4 + J\varphi + \text{NLT}\,, \tag{32}$$

where NLT denotes « nonlocal terms ». All parameters in eq. (32) depend on Π and are functionals of $h(\boldsymbol{x})$ the continuum limit of h_i. On the other hand, Π does not enter the original Hamiltonian (18) and it has to be determined through eq. (19) which in the present context assumes the form

$$\Pi = \left.\frac{\delta F}{\delta h(\boldsymbol{x})}\right|_{h(\boldsymbol{x})=0}, \tag{33}$$

where F is the generating functional of the connected diagrams. Moreover, it is worth pointing out that $\langle\varphi\rangle$ is not the order parameter Π, since $J(\boldsymbol{x})$ is not equal to $h(\boldsymbol{x})$. One has then

$$\Pi = \int \frac{\delta F}{\delta J(\boldsymbol{x}')} \left.\frac{\delta J(\boldsymbol{x}')}{\delta h(\boldsymbol{x})}\right|_{h(\boldsymbol{x})=0} \mathrm{d}\boldsymbol{x}' = \int \langle\varphi(\boldsymbol{x}')\rangle \left.\frac{\delta J(\boldsymbol{x}')}{\delta h(\boldsymbol{x})}\right|_{h(\boldsymbol{x})=0} \mathrm{d}\boldsymbol{x}' . \tag{34}$$

Equation (34) is just the consequence of the local rotation (23). The solution of eq. (34) looks like a very impressive task, but we want to emphasize, as a conclusion, that the field Hamiltonian (32) describes the system in the low-temperature broken-symmetry phase (at least when the condition (2) is satisfied).

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