

Analytical results for the Coqblin-Schrieffer model with generalized magnetic fields

V. V. Bazhanov,^{1,2} S. L. Lukyanov,^{3,4} and A. M. Tsvetik⁵

¹*Department of Theoretical Physics, Research School of Physical Sciences and Engineering, Australian National University, Canberra, ACT 0200, Australia*

²*Research Institute for Mathematical Sciences, Kyoto University, Kyoto 606-8502, Japan*

³*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08855-0849, USA*

⁴*L. D. Landau Institute for Theoretical Physics, Chernogolovka 142432, Russia*

⁵*Department of Physics, Brookhaven National Laboratory, Upton, New York 11973-5000, USA*

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Using the approach alternative to the traditional thermodynamic Bethe ansatz, we derive analytical expressions for the free energy of Coqblin-Schrieffer model with arbitrary magnetic and crystal fields. In the Appendix we calculate the zero-temperature magnetic susceptibility for two concrete crystal-field patterns. One of the patterns describes the field generated crossover from the SU(4) to the SU(2) symmetry in the SU(4)-symmetric model.

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The advances of nanotechnology have given an additional weight to the old problem of Kondo effect. Artificially manufactured structures such as quantum dots emulate the behavior of “natural” magnetic impurities though on different energy scales. Using technological means one can widely vary the parameters of the dots thus getting an access to previously experimentally unexplored regions of the phase diagram.

The most physically transparent situation corresponds to the case when magnetic impurity (or quantum dot) has a perfect symmetry. This, however, is rarely achieved in real systems due to the presence of the crystalline lattice. Let us consider, for instance, magnetic impurities made of rare-earth magnetic ions of Ce and Yb. In the presence of a strong spin-orbital coupling, an f^1 (Ce) or f^{13} (Yb)-orbital is characterized by the total angular momentum j ($j=5/2$ for Ce and $7/2$ for Yb) such that an isolated ion has the SU(n) symmetry with $n=2j+1$. In the crystalline environment this symmetry is broken. The interplay of these effects with the Kondo screening can be studied using the Coqblin-Schrieffer model¹

$$\mathbf{H} = \sum_{k,a} k c_{k,a}^\dagger c_{k,a} + \frac{J}{V} \sum_{k,k'} c_{k,a}^\dagger c_{k',b} \mathbf{f}_b^\dagger \mathbf{f}_a + \sum_a H_a \mathbf{f}_a^\dagger \mathbf{f}_a, \quad (1)$$

where $c_{k,a}^\dagger$ and $c_{k,a}$ are creation (annihilation) operators of the conduction electrons partial harmonics with the angular momentum projection $m=j+1-a$ ($a=1, \dots, n$), \mathbf{f}_a^\dagger and \mathbf{f}_a operators describe the impurity spin, and V is the volume of the system. The generalized magnetic field H_a originates from crystal fields inherent to the material and the external magnetic field. Since Hamiltonian (1) commutes with the operator

$$\mathbf{q} = \sum_{a=1}^n \mathbf{f}_a^\dagger \mathbf{f}_a,$$

one can assume without loss of generality that

$$\sum_{a=1}^n H_a = 0. \quad (2)$$

Note that the cases described above correspond to the sector of the Coqblin-Schrieffer model with the occupation number $q=1$.

Since model (1) has a linear spectrum, it has to be equipped with the ultraviolet (UV) cutoff Λ and a consistent removal of the UV divergences requires that the “bare” coupling $g_0 = nJ\rho(0)$ [here $\rho(0)$ is the conduction electron density of states at the chemical potential] be given certain dependence of the cutoff momenta (see, e.g. in Ref. 2):

$$\Lambda \frac{dg_0}{d\Lambda} = -g_0^2 + \frac{g_0^3}{n} + \dots \quad (3)$$

Equation (3) shows that for positive g_0 the Coqblin-Schrieffer model acquires a physical energy scale, the Kondo temperature

$$T_K \sim \Lambda g_0^{1/n} e^{-1/g_0}, \quad (4)$$

and renormalization trades the bare coupling constant g_0 for the renormalization group invariant scale T_K . Therefore the partition functions of the model in the sector with a given occupation number q , Z_q , actually depends on the dimensionless combinations T/T_K and H_a/T_K . Of course, formula (4) does not specify the physical energy scale uniquely and in order to define T_K unambiguously we shall impose the conventional normalization condition³

$$\lim_{T \rightarrow 0} C_1(T)/T|_{H_a=0} = \frac{\pi}{3} \frac{n-1}{T_K}, \quad (5)$$

where $C_1(T) = T(\partial^2/\partial T^2)(T \log Z_{q=1})$ is the heat capacity of the impurity in the sector with the occupation number $q=1$.

If the fields are weak in comparison with the Kondo temperature (5), the behavior of the system is governed by $T_K^{(n)}$ [the Kondo temperature of the fully SU(n)-symmetric

model] which for rare earth impurities may be as large as several hundred degrees. On the other extreme, if the generalized magnetic fields exceed $T_K^{(n)}$ and break down the degeneracy to one Kramers doublet, one gets the Kondo temperature of the order of several degrees. As an illustration let us estimate the new Kondo temperature for the case when the original $SU(n)$ symmetry is broken down to $SU(m)$ by the fields $H_1, \dots, H_{n-m} \gg T_K^{(n)}$. The estimate is easy if all the fields H_1, \dots, H_{n-m} are of the same order \bar{H} . Since $\ln T_K^{(n)} \sim -1/n J\rho(0)$, $\ln T_K^{(m)} \sim -1/m J\rho(0)$, and the dimensionless ground state energy depends only on $H_a/T_K^{(n)}$, we conclude that the resulting Kondo temperature is^{4,5}

$$T_K^{(m)} \sim \bar{H} (T_K^{(n)}/\bar{H})^{n/m}, \quad (6)$$

which may easily constitute a scale vastly different from the Kondo temperature of the unperturbed model. It is clear that the detailed behavior in this crossover interval depends on the field ratios H_a/H_b and it would be highly desirable to have analytical tools to handle a situation with an arbitrary pattern of fields.

Historically the thermodynamics of the Coqblin-Schrieffer model has been examined by the method of thermodynamic Bethe ansatz (TBA) (Refs. 3,5–8). Unfortunately the TBA equations corresponding to Eq. (1) are rather complicated to be studied analytically, and until now the majority of results have been obtained by means of their numerical integration (see Ref. 9 and references therein).

This work is based on the approach alternative to the TBA. Here we just outline major steps of our analysis and refer the reader to the papers^{10–12} where the method itself was developed (see also important works in Ref. 13). Let us make some remarks on the general spirit of the approach. It uses the fact that integrable impurity models in general and the Coqblin-Schrieffer model in particular can be mapped to the $(1+1)$ -dimensional bulk conformal field theory (CFT) with a nonconformal boundary interaction (see e.g. in Ref. 14). From this point of view, Eq. (1) belongs to the class of exactly solvable boundary theories such that the associated boundary state commutes with the infinite set of mutually commutative local integrals of motion of the bulk system. As a matter of fact, one may say that the boundary state “generates” this set in the sense that it admits the asymptotic large distance expansion in terms of these local integrals. More precisely, the Hilbert space of the bulk CFT associated with Eq. (1) can be classified in accordance with the WA_{n-1} -algebra¹⁵ with the central charge $c=n-1$ and the corresponding boundary state commutes with the set of local integrals of motion introduced in Ref. 15.

In the approach adopted in this paper, the amplitudes of the boundary state are related to monodromy characteristics of certain ordinary linear differential equations. The key ingredient is the equation of the form,

$$[(-i\partial_v + h_1) \dots (-i\partial_v + h_n) - e^{n\theta} e^{v/n}] \Psi = 0, \quad (7)$$

where θ and h_a are some (complex) parameters. For $\text{Im}(\theta) = \pi/2$ the equation admits a solution which is specified unambiguously by the following asymptotic as $v \rightarrow +\infty$:

$$\Psi_0(v, \theta) \rightarrow (-ie^{\theta} v^{1/n} e^{v/n})^{-(n-1/2)} \times \exp\left\{ie^{\theta} \left(C + \int_0^v du u^{1/n} e^{u/n}\right)\right\}. \quad (8)$$

Here C is an arbitrary constant, whose explicit value is not essential for our purposes. Note that Eq. (7) is invariant under the transformation, $\theta \rightarrow \theta + 2\pi i/n$, whereas the asymptotic (8) is not. Hence the analytic continuations of Ψ_0 ,

$$\Psi_q(v, \theta) = \Psi_0(v, \theta + 2\pi i q/n), \quad (9)$$

with integers q , generate new solutions of Eq. (7). It is possible to show that the Wronskian $W[\Psi_0, \Psi_1, \dots, \Psi_{n-1}]$ does not vanish, so that the set $\{\Psi_q\}_{q=0}^{n-1}$ is a fundamental system of solutions of Eq. (7). By virtue of this fact, solution (9) with $q=n$ can be decomposed as

$$\Psi_n(v, \theta) = \sum_{q=0}^{n-1} (-1)^{n-q-1} Z_q(\theta + i\pi q/n) \Psi_q(v, \theta). \quad (10)$$

Following the line of arguments similar to that of Refs. 10,11, it is possible to show that if the parameters θ and h_a are identified with the dimensionless parameters of the Coqblin-Schrieffer model

$$e^{\theta} = \frac{1}{2n^{1/n} \Gamma(1/n)} \frac{T_K}{T}, \quad h_a = \frac{H_a}{2\pi T}, \quad (11)$$

then the function $Z_q(\theta)$ appearing in Eq. (10) coincides with the analytic continuation of the partition function of this model Z_q for the sector with occupation number q .

The subject of our current interest is the free energies

$$\mathcal{F}_q = -T \log(Z_q) \quad (12)$$

at the low temperature limit. In particular we study vacuum energies $\mathcal{E}_q = \mathcal{F}_q|_{T=0}$. It can be worked out by means the semi-classical Wentzel, Kramer, and Brillouin (WKB) approximation for Eq. (7). The leading terms in the WKB expansion of the solution Ψ_0 (8) read

$$\Psi_0(v, \theta) \simeq (-iX(e^{\theta} v^{1/n} e^{v/n}))^{-(n-1/2)} \times \exp\left\{ie^{\theta} \left(C + \int_0^v du u^{1/n} e^{u/n}\right) - i \int_v^{+\infty} du (X(Y) - Y) \Big|_{Y=e^{\theta} u^{1/n} e^{u/n}}\right\}. \quad (13)$$

Here $X=X(Y)$ is the solution of the algebraic equation

$$Y^n = (X + h_1) \dots (X + h_n), \quad (14)$$

such that

$$X(Y) \rightarrow Y \quad \text{as} \quad Y \rightarrow \infty. \quad (15)$$

In fact, $X=X(Y)$ is a multi-valued function of the argument Y and Eq. (15) uniquely specifies its branch for a sufficiently large Y . The latter solution admits a convergent $1/Y$ -power series expansion found by Lagrange:¹⁶

$$X(Y) = Y + \frac{1}{n} \sum_{\substack{k=1 \\ k \neq 0(\text{mod } n)}}^{\infty} I_k(h_1, \dots, h_n) Y^{-k}. \quad (16)$$

Here I_k are symmetric polynomials given by

$$I_k(h_1, \dots, h_n) = \sum_{\substack{\alpha_1, \dots, \alpha_{n-1} \geq 0 \\ 2\alpha_1 + 3\alpha_2 + \dots + n\alpha_{n-1} = k+1}} \frac{(-1)^{\alpha_1 + \dots + \alpha_{n-1}} \Gamma(\alpha_1 + \dots + \alpha_{n-1} - k/n)}{\alpha_1! \alpha_2! \dots \alpha_{n-1}!} \frac{\Gamma(1 - k/n)}{\Gamma(1 - k/n)} G_2^{\alpha_1} G_3^{\alpha_2} \dots G_n^{\alpha_{n-1}}, \quad (17)$$

where we use the following notation for the elementary symmetric polynomials G_k :

$$G_k = \sum_{1 \leq a_1 < a_2 < \dots < a_k \leq n} h_{a_1} \dots h_{a_k}. \quad (18)$$

Note that according to constraint (2), we have set $G_1 = 0$, and also $G_2 = -\frac{1}{2} \sum_{a=1}^n h_a^2$.

Using Lagrange formulas (16) and (13) it is possible to show that the vacuum energies admit the following weak-field expansion¹⁷

$$\begin{aligned} \mathcal{E}_q = E_0 \sin\left(\frac{\pi q}{n}\right) + \frac{T_K}{n} \\ \times \sum_{\substack{k=1 \\ k \neq 0(\text{mod } n)}}^{\infty} C_k \sin\left(\frac{\pi k q}{n}\right) I_k\left(\frac{H_1}{2\pi T_K}, \dots, \frac{H_n}{2\pi T_K}\right), \end{aligned} \quad (19)$$

where

$$C_k = 2^{k+1} k^{k/n} \Gamma^k(1/n) \Gamma(-k/n).$$

The first term in Eq. (19) is the vacuum energy for zero fields and the value of $E_0 \sim T_K$ is related to the choice of the constant \mathcal{C} in Eq. (8).¹⁸ Note that I_k (17) are homogeneous symmetric polynomials of the variables h_a of the degree $k+1$, i.e.,

$$I_k(\lambda h_1, \dots, \lambda h_n) = \lambda^{k+1} I_k(h_1, \dots, h_n), \quad (20)$$

so Eq. (19) can be considered as a power series expansion in $\bar{H}/(2\pi T_K)$, where $\bar{H} = \sqrt{1/n \sum_{a=1}^n H_a^2}$. Thus if the fields are weak in comparison with the Kondo temperature the behavior of the system is governed by convergent series (19). At the same time the series has a finite convergence radius, and defines the multi-valued function of complex variable \bar{H} (see the Appendix for examples).

We have also examined the structure of the low temperature expansion of the free energy (12) and found the following asymptotic series:

$$\begin{aligned} \mathcal{F}_q = E_0 \sin\left(\frac{\pi q}{n}\right) + \frac{T_K}{n} \\ \times \sum_{\substack{k=1 \\ k \neq 0(\text{mod } n)}}^{\infty} C_k \sin\left(\frac{\pi k q}{n}\right) \mathbb{I}_k\left(\frac{H_1}{2\pi T}, \dots, \frac{H_n}{2\pi T}\right) \left(\frac{T}{T_K}\right)^{k+1} \\ + O(T^\infty). \end{aligned} \quad (21)$$

Here the numerical coefficients C_k are the same as in Eq. (19) and $\mathbb{I}_k(h_1, \dots, h_n)$ is the symmetric polynomial of the degree k of the form

$$\mathbb{I}_k = I_k + \sum_{l=0}^k I_k^{(l)}, \quad (22)$$

where I_k is given by Eq. (17) and $I_k^{(l)} = I_k^{(l)}(h_1, \dots, h_n)$ are some homogeneous symmetric polynomials of the degree $0 \leq l \leq k$. Currently the polynomials \mathbb{I}_k are not known in a closed form for arbitrary k . Nevertheless, they admit a simple algebraic description. As has been mentioned before, the boundary state associated with the Coqblin-Schrieffer model commutes with the infinite set of mutually commutative integrals of motion for the WA_{n-1} -algebra with the central charge $c = n - 1$. It turns out that the polynomials \mathbb{I}_k appearing in Eq. (21) coincide with vacuum eigenvalues of these conserved charges. Therefore they can be calculated purely algebraically for any finite k . In particular we found

$$\begin{aligned} \mathbb{I}_1 &= -G_2 + \frac{n-1}{24}, \quad \mathbb{I}_2 = -G_3, \\ \mathbb{I}_3 &= -G_4 + \frac{n-3}{2n} G_2^2 - \frac{n-3}{8n} G_2 + \frac{3(n-1)(n-3)}{640n}, \\ \mathbb{I}_4 &= -G_5 + \frac{n-4}{n} G_3 G_2 - \frac{n-4}{3n} G_3. \end{aligned} \quad (23)$$

Here G_k are elementary symmetric polynomials (18). Note that for the physically interesting case of the magnetic field configuration

$$h_a = h(j+1-a), \quad j = \frac{n-1}{2}, \quad (24)$$

all the polynomials I_k with even k vanish, whereas using Eq. (23) one has

$$I_1 = \frac{n-1}{24} [n(n+1)h^2 + 1],$$

$$I_3 = \frac{(n-1)(n-3)}{1920n} [n^2(n+1)(n+3)h^4 + 10n(n+1)h^2 + 9]. \quad (25)$$

In conclusion let us just repeat the basic results of the paper. We have outlined a method which allows to extract analytical results for the thermodynamics of Coqblin-Schrieffer model in the presence of magnetic and crystal fields. The general formulas drastically simplify for the SU(4) model (see the Appendix).

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APPENDIX

In this appendix we illustrate the expansion (19) using two examples.

Our first example is related to the case $n=4$. Let us consider the following configuration of the generalized magnetic fields

$$H_1 = -H_4, \quad H_2 = -H_3, \quad (A1)$$

with $H_1 \geq H_2 \geq 0$. In this case Eq. (14) is especially simple and can be written in the form

$$Y^4 = (X^2 - h_1^2)(X^2 - h_2^2). \quad (A2)$$

Its solution $X = X(Y)$ satisfying Eq. (15) reads explicitly

$$x = y \sqrt{\sqrt{1 + \epsilon/y^4} + 1/y^2}, \quad (A3)$$

where $y = Y/\bar{h}$, $x = X/\bar{h}$, and

$$\bar{h} = \sqrt{\frac{h_1^2 + h_2^2}{2}}, \quad \epsilon = \left(\frac{h_1^2 - h_2^2}{h_1^2 + h_2^2} \right)^2.$$

All even coefficients I_{2l} in series (16) vanish now, whereas I_{2l-1} can be expressed in terms of the hypergeometric function

$$I_{2l-1} = 2(-1)^{l-1} \frac{\Gamma(l-1/2)}{\sqrt{\pi} l!} \bar{h}_2^{2l} F_1 \left(-\frac{l}{2}, \frac{1}{2} - \frac{l}{2}, \frac{3}{4} - \frac{l}{2}; \epsilon \right). \quad (A4)$$

Combining this equation with Eq. (19) one obtains,

$$\begin{aligned} \mathcal{E}_q &= E_0 \sin\left(\frac{\pi q}{4}\right) + \frac{T_K}{\sqrt{2}\Gamma(1/4)} \sum_{l=1}^{\infty} \frac{(-1)^l}{l!} (2l-1)^{(l/2-5/4)} \\ &\times \Gamma\left(\frac{l}{2} + \frac{1}{4}\right) \frac{\sin(\pi(2l-1)q/4)}{\sin(\pi(2l-1)/4)^2} \\ &\times F_1\left(-\frac{l}{2}, \frac{1}{2} - \frac{l}{2}, \frac{3}{4} - \frac{l}{2}; \epsilon\right) \left(\frac{\Gamma(1/4)\sqrt{2}\bar{H}}{\pi T_K}\right)^{2l}, \quad (A5) \end{aligned}$$

with

$$\bar{H} = \sqrt{\frac{H_1^2 + H_2^2}{2}}, \quad \epsilon = \left(\frac{H_1^2 - H_2^2}{H_1^2 + H_2^2} \right)^2 \leq 1.$$

Note that Eq. (A5) can be rewritten in the form of a convergent integral which is useful for an analytical continuation of the power series expansion outside its convergence disk,

$$|\bar{H}/T_K| < \frac{\pi e^{-1/4}}{\sqrt{2}\Gamma(1/4)} \min[\epsilon^{-1/4}, (1-\epsilon)^{-1/4}].$$

Explicitly one has ($q=1,2,3$),

$$\begin{aligned} \mathcal{E}_q &= E_0 \sin\left(\frac{\pi q}{4}\right) + \bar{H} \sin\left(\frac{\pi q}{4}\right) \\ &\times \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (i\omega + 0)^{i\omega-1} \frac{\Gamma(-1/2-2i\omega)}{\Gamma(1/2-i\omega)} \left(\frac{2\Gamma(1/4)\bar{H}}{\pi T_K}\right)^{4i\omega} \\ &\times F_1\left(\frac{1}{4} - i\omega, -\frac{1}{4} - i\omega, \frac{1}{2} - i\omega; \frac{1}{2} - (-1)^q \frac{1-2\epsilon}{2}\right). \quad (A6) \end{aligned}$$

It is particularly illuminating to extract the Kondo temperature from this expression for the SU(2) Coqblin-Schrieffer model to compare it with Eq. (6). The Kondo temperature $T_K^{(2)}$ can be extracted from the magnetic susceptibility in the limit when one of the fields is very large. Since the energy depends on two fields H_1 and H_2 , one has to be careful in choosing the right direction of differentiation. The right choice of variables is $H_{\pm} = H_1 \pm H_2$ such that $\partial\mathcal{E}_1/\partial H_- = 0$ at $H_- = 0$. Then at $H_+ \rightarrow 2\bar{H} \gg T_K$, $H_- \rightarrow 0$ we obtain for $q=1$ the following expression for the magnetic susceptibility:

$$\chi = -\frac{\partial^2 \mathcal{E}_1}{\partial H_-^2} \Big|_{H_- = 0} \Big|_{H_+ = 2\bar{H}} \rightarrow \frac{1}{2\pi T_K^{(2)}}, \quad T_K^{(2)} = \frac{\pi^{3/2}}{\sqrt{8}\Gamma^2(1/4)} \frac{T_K^2}{\bar{H}}. \quad (A7)$$

The above expression for the effective Kondo temperature is a particular case of Eq. (6) for $n=4, m=2$.

Our second example is related to the case of an arbitrary integer n . In Ref. 3, the vacuum energy \mathcal{E}_1 was found for the following fields configuration:

$$H_a = \sqrt{2}\bar{H} \cos\left(\frac{\pi(2a-1)}{2n}\right). \quad (\text{A8})$$

For this pattern Eq. (14) is expressed in terms of the Chebyshev polynomials $T_n(x) = \cos[n \arccos(x)]$

$$y^n = 2^{1-n/2} T_n(x/\sqrt{2}), \quad (\text{A9})$$

where $y = Y/\bar{h}$, $x = X/\bar{h}$. Therefore

$$x = y_2 F_1\left(-\frac{1}{2n}, \frac{n-1}{2n}, \frac{n-1}{n}; \frac{2^{2-n}}{y^{2n}}\right) + \frac{1}{2y^2} F_1\left(\frac{1}{2n}, \frac{n+1}{2n}, \frac{n+1}{n}; \frac{2^{2-n}}{y^{2n}}\right), \quad (\text{A10})$$

and nonvanishing coefficients in Eqs. (16) and (19) are I_{2nl-1} ($l=1,2,\dots$) and I_{2nl+1} ($l=0,1,2,\dots$):

$$I_{2nl+\sigma} = \sigma \frac{\Gamma\left(\frac{\sigma}{n} + 2l\right)}{l! \Gamma\left(1 + \frac{\sigma}{n} + l\right)} \left(\frac{\bar{h}}{\sqrt{2}}\right)^{2ln+1+\sigma}, \quad \sigma = \pm 1. \quad (\text{A11})$$

As in the first example, the vacuum energies (19) can be written in the form of convergent integral:³

$$\mathcal{E}_q = E_0 \sin\left(\frac{\pi q}{n}\right) + \frac{\sqrt{2}\bar{H} \sin(\pi q/n)}{4\pi n} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (i\omega + 0)^{i\omega-1} \times \Gamma\left(-\frac{1}{2n} - \frac{i\omega}{2}\right) \Gamma\left(\frac{1}{2n} - \frac{i\omega}{2}\right) \left(\frac{n^{1/n} \Gamma(1/n) \bar{H}}{\pi \sqrt{2} T_K}\right)^{i\omega}. \quad (\text{A12})$$

It is easy to check that this equation for $n=4$ is in agreement with (A6) provided $\epsilon = 1/2$.

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¹⁸According to the $1/n$ -expansion of Ref. 2, $E_0/T_K = 1 + O(n^{-2})$.