Mean-field method for handling null constraints on positive-definite operators

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We present an approach for studying systems with hard constraints that certain positive-definite operators must vanish. The difficulty with mean-field treatments of such cases is that imposing that the constraint is zero only in average is problematic for a quantity that is always positive. We reformulate the hard constraints by adding an auxiliary system such that some of the states to be projected out from the total system are at finite negative energy and the rest at finite positive energy. This auxiliary system comes with an extra coupling that is unfixed, and that parametrizes a whole family of mean-field theories. We argue that this variational-type parameter for the family of mean-field theories should be fixed by matching a given experimental observation, with the quality of the resulting mean-field approximation measured by how it fits other data. We test these ideas in the well-understood single-impurity Kondo problem, where we fix the parameter via the T_K obtained from the magnetic susceptibilty value, and score the quality of the approximation by its predicted Wilson ratio.

I. INTRODUCTION

One of the key theoretical challenges in condensed matter physics is to understand systems with strong correlations, when interactions become larger than the kinetic energy dispersion bandwidth. Physical systems which fall in this important class include: the cuprate superconductors, where strong interactions between electrons in copper's 3d shells lead to an antiferromagnetic Mott insulator at half-filling and superconductivity upon hole doping; heavy-electron compounds where localized d and f orbitals of rare earth and transition metal atoms interact with itinerant electrons, leading to a renormalization of the electron mass by as much as a thousand times; and systems of cold atomic gases, where interactions may be tuned by a Feshbach resonance to realize strongly interacting multispecies systems [1–5, 9, 10, 16, 17]. In these and other examples of strongly correlated systems of interest in modern condensed matter physics, it is customary to encounter a broad range of energy scales that make any theoretical study a tall order. One can often make substantial progress by producing effective models where the largest energy scales are "projected out"; namely, the system is assumed to be in the lowest energy states of these large energy terms, thus introducing strict conditions (or constraints) in the effective models. These constraints lead to effective models such as the t-J model, the Heisenberg model, and the Kondo model, to name a few.

In this work we propose a method, which we call the soft constraint, to study systems where the constraint is that a positive-definite operator anihilates the physical states. A mean-field treatment of the constraint, where it is satisfied in average, not identically, is that the average is already lower-bounded by zero, because of the positive-definiteness of the operator. Therefore, the mean-field theory would be biased towards failure. Here we propose a method to circunvent this problem: we introduce an auxiliary degree of freedom with its own constraint, and construct a combined constraint that is satisfied only when both the original and new constraints are satisfied. The new quantity is no longer positive definite, and hence the combined constraint can now be satisfied only in average. This method comes with an additional parameter than can be varied freely. We thus have not one, but instead a family of theories that, when treated exactly, reproduce the correct constraints. When treated within a mean-field approximation, the family of therories become different approximations to the same physical problem. We propose to fix the value of the parameter as follows: we choose one physical observable, and find the value of the "variational mean-field" parameter to best match the observable. The usefulness of the approximation with this fixed parameter can be measured by how it fits other observables. We choose as a benchmark the single-impurity Kondo problem, where we fix the parameter via the T_K obtained from the magnetic susceptibilty value, and grade the quality of the approximation by the deviation of the predicted Wilson ratio from the exact Bethe Ansatz result.

The introduction of the auxiliary system allows us to impose the zero-average condition in the combined operator, but as we shall see, the combined operator is often not quadratic. To deal with quartic terms, we use the Kotliar-Ruckenstein approach. The combination of these two methods produces better results then the conventional Read-Newns meanfield for the Kondo model [1] for the Wilson ratio, and it reproduces the width of the Abrikosov-Suhl resonance to two loop level for the Kondo RG [1].

In addition to the Kondo problem, we show that the method gives the exact density of states for the infinite U Anderson model. In fact, we use this system as a simple way to first present, in section II, the basics of the soft-constraint method. Other systems that could be studied using these techniques include hard-core bosons, spinor condensates, t-J, Heisenberg, two-channel Kondo and two-channel Anderson models.

II. A FIRST EXAMPLE: THE INFINITE U ANDERSON MODEL

As a first simple example of the soft constraint method we would like to present a soft constraint formulation of the infinite U Anderson model focusing on the case where there is one spin 1/2 impurity. The Hamiltonian for the Anderson model is given by:

$$H_A = U n_\uparrow n_\downarrow + \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma} c_{k,\sigma} + V \sum_{k,\sigma} c^\dagger_{k,\sigma} f_\sigma + h.c. \tag{1}$$

Where the limit $U \to \infty$ is understood. We will consider an auxiliary system unrelated to the impurity which is used to satisfy the soft constraint. A variety of auxiliary systems are possible, slave bosons, slave fermions, slave spins and even slave compound systems; we shall focus on the case of the slave fermion h. Let

$$H = H_A + H' \tag{2}$$

With

$$H' = \tilde{U} h^\dagger h \tag{3}$$

We will consider the case when $\tilde{U} \to \infty$. in this case we are constraining all the fermions to lie in their ground state so we are effectively multiplying **(CCh - ???)** the initial Anderson model H_A by one. We have two hard constrains in this system:

$$\begin{aligned} h^\dagger h &= 0 \\ n_\uparrow n_\downarrow &= 0 \end{aligned} \tag{4}$$

We would like to replace these with an equivalent constraint where

$$\tilde{\Pi} = n_\uparrow n_\downarrow - K h^\dagger h = 0 \tag{5}$$

Here $K > 0$ and $K \neq 1$. As such the partition function of the Anderson model is given by:

$$\begin{aligned} Z = e^{-\beta H_A} &= \prod_n \left\{ e^{-\varepsilon_n \tilde{H}_A} \prod_s \tilde{\Pi}_s \right\} \\ &= \frac{1}{N} \prod_n e^{-\varepsilon_n \tilde{H}_A} \prod_s \int d\lambda_{s,n} e^{-\varepsilon_n \lambda_{s,n} \left(n_{s,\sigma} n_{s,\sigma'} - K h^\dagger h \right)} \end{aligned} \tag{6}$$

In this identity K is an arbitrary parameter. We now take the stationary phase with respect to the parameter $\lambda_n \to \lambda^0$. In which case we get the equation:

$$\frac{dZ}{d\lambda_n} = 0 \Rightarrow \left\langle n_\uparrow n_\downarrow - K h^\dagger h \right\rangle = 0 \tag{7}$$

We would like to note that if we had not introduced the slave fermion h or equivalently $K = 0$ we would not have obtained a solvable meanfeld as $n_\uparrow n_\downarrow$ is a positive semidefinite operator. For our next step we can maximize the partition function with respect to K, from which we get that:

$$\frac{dZ}{dK} = 0 \Rightarrow \lambda^0 \left\langle h^\dagger h \right\rangle = 0 \tag{8}$$

From which we get that the optimum meanfield (with the largest partition function) is given by $\lambda^0 = 0$. This means that at meanfield the partition function for the Anderson model is given by:

$$Z = e^{-\beta H_A} = \prod_n \left\{ e^{-\varepsilon_n \tilde{H}_A} \prod_s \tilde{\Pi}_s (\lambda_s = 0) \right\} = \frac{1}{N} \prod_n e^{-\varepsilon_n \tilde{H}_A} \tag{9}$$

That is its the partition function of the model with $U = 0$. For the case of the single impurity with energy E_f it is known that the physics of the non-interacting model is controlled by the physics of the single impurity (with no free fermions) where the action is given by:

$$S_A = \sum_n \sum_\sigma (-i\omega_n + E_f - i\Delta sgn(\omega_n)) f^\dagger_\sigma f_\sigma \tag{10}$$

where $\Delta = \pi \left| V^2 \right| \rho$, where ρ is the density of states of the free fermions. the density of states for the impurity is given by:

$$\rho_s(\omega) = \frac{1}{\pi} \frac{\Delta}{\Delta^2 + (\omega - E_f)^2} \tag{11}$$

This approach does not capture the Abrikosov-Suhl resonance [1] but provides a good starting point when considering the density of states near the resonance near $-|E_f|$. We will therefore keep λ general as every λ produces a proper meanfield and study the Abrikoson-Suhl resonance [1] using this more general formulation.

III. THE KONDO MODEL

To study the physics of the Abrikoson-Suhl resonance in its simplest form and to study the soft constraint for another model we will now switch gears and study the Kondo model which is related to the infinite U Anderson model [1]. The Kondo model is given by the following Hamiltonian:

$$H_{Kondo} = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + J \sum_k \vec{S}_k \cdot \vec{S}_0$$

Where $\vec{S}_0$ is a localized spin located at the origin. For a uniform density of states for the fermions $c_{k,\sigma}$ this model has an exact solution by the Bethe ansatz leading to exact results for the magnetic susceptibility, density of states and heat capacity [8, 9], we will strive to reproduce these results using a simpler meanfield method. As a first step let us consider the Read-Newns formulation of the single impurity Kondo model, with Lagrangian given by:

$$L_{RN} = \sum_{k,\sigma} c^\dagger_{k\sigma}\left(\frac{d}{d\tau}+\epsilon_k\right)c_{k\sigma} + \sum_\sigma f^\dagger_\sigma\left(\frac{d}{d\tau}+\lambda_{RN}\right)f_\sigma - \sum_{k,\sigma}\left\{\bar{V}\left(c^\dagger_{k,\sigma}f_\sigma\right)+V\left(f^\dagger_\sigma c_{k,\sigma}\right)\right\}+2\frac{V\bar{V}}{J}-\lambda_{RN} \quad (12)$$

where λ_{RN} is a multiplier that enforces single occupancy $\sum_\sigma f^\dagger_\sigma f_\sigma = 1$ in the spin-1/2 fermion representation of the magnetic impurity.

At mean field level, the Read-Newns formulation predicts a Kondo temperature

$$T_K \sim D\exp\left(-\frac{1}{J\rho}\right), \quad (13)$$

where D is the band width. The exact Kondo temperature however is given by:

$$T_K \sim D\sqrt{J\rho}\exp\left(-\frac{1}{J\rho}\right), \quad (14)$$

where the factor of $\sqrt{J\rho}$, missing in the mean field result, can easily lead to a substantial correction to the value of T_K. This discrepancy has measurable consequences, since for instance the Kondo temperature is directly related to the susceptibility:

$$\chi \sim \frac{(g\mu_B)^2}{T_K}. \quad (15)$$

Furthermore the meanfield Wilson ratio is one, indicating that the meanfield also greatly underestimates the heat capacity.

IV. SOFT CONSTRAINT APPROACH

Here we consider a different approach, which starts by re-writing the condition $\sum_\sigma f^\dagger_\sigma f_\sigma = 1$ as

$$(1-n_\uparrow-n_\downarrow)^2 = n_\uparrow n_\downarrow + (1-n_\uparrow)(1-n_\downarrow) = 0. \quad (16)$$

Whereas this approach is identical to the Read-Newns formulation in the exact Lagrangian, it must be handled differently at mean field level. Indeed, the constraint is expressed now in terms of a positive semi-definite function that needs to be set to zero, and this cannot be achieved at mean field level as it would necessarily give a diverging mean field parameter when solved self-consistently. We introduce instead an auxiliary non-interacting fermionic Hilbert space that is constrained to be trivially empty: $h^\dagger h = 0$. For any non-integer positive parameter K, we can then combine the constraints in the original problem and in the auxiliary fermions by imposing:

$$n_\uparrow n_\downarrow + (1-n_\uparrow)(1-n_\downarrow) - K\,h^\dagger h = 0. \quad (17)$$

Notice that this is exactly equivalent to enforcing $n_\uparrow n_\downarrow + (1-n_\uparrow)(1-n_\downarrow) = 0$ and $h^\dagger h = 0$ separately. However, we are now able to treat the combined constraint at mean field level and look for finite parameters at saddle point.

The soft constraint Lagrangian can then be written as

$$\begin{aligned} L_{SC} = &\sum_{k,\sigma} c^\dagger_{k\sigma}\left(\frac{d}{d\tau}+\epsilon_k\right)c_{k\sigma} + \sum_\sigma f^\dagger_\sigma \frac{d}{d\tau} f_\sigma \\ &- \sum_\sigma\left\{\bar{V}\sum_k\left(c^\dagger_{k,\sigma}f_\sigma\right)+V\left(f^\dagger_\sigma c_{k,\sigma}\right)\right\}+2\frac{V\bar{V}}{J} \\ &+\lambda_{SC}\left[n_\uparrow n_\downarrow + (1-n_\uparrow)(1-n_\downarrow) - K\,h^\dagger h\right] \\ &+ h^\dagger\frac{d}{d\tau}h. \end{aligned} \quad (18)$$

Notice that Eq.(18) is not a mean field Lagrangian because of the terms $\propto n_\uparrow n_\downarrow$. It is possible to use the Kotliar Rukenstein formulation of the Anderson model to convert our Kondo path integral into a mean field [12, 17]. We recall that the Kotliar Rukenstein slave formulation uses four slave bosons, e, d and p_σ. These represent the empty, doubly occupied and spin up and spin down singly occupied states. Immediately one needs to impose the constraint:

$$e^\dagger e + \sum_\sigma p^\dagger_\sigma p_\sigma + d^\dagger d = 1, \quad (19)$$

that there is one physical state. Furthermore to ensure that the state of the fermion is correlated with the state of the boson, one needs to impose two constraints, one per spin species:

$$f^\dagger_\sigma f_\sigma = p^\dagger_\sigma p_\sigma + d^\dagger d. \quad (20)$$

The electron operator is then given by:

$$f_\sigma \to z_\sigma f_\sigma, \qquad z_\sigma = e^\dagger p_\sigma + p^\dagger_{-\sigma} d. \quad (21)$$

It is also conventional to transform

$$z_\sigma \to \left(1-d^\dagger d - p^\dagger_\sigma p_\sigma\right)^{-1/2} z_\sigma \left(1-e^\dagger e - p^\dagger_{-\sigma}p_{-\sigma}\right)^{-1/2}. \quad (22)$$

The operators z_σ move between the four allowed boson states while f_σ moves between the fermion states, this identity insures that the states of the bosons and fermions remain correlated and that the constraint in Eq.(20) is satisfied. The Lagrangian for this formulation is given by:

$$\begin{aligned} &e^\dagger\frac{d}{d\tau}e + d^\dagger\frac{d}{d\tau}d + \sum_\sigma p^\dagger_\sigma\frac{d}{d\tau}p_\sigma + \sum_\sigma f^\dagger_\sigma\frac{d}{d\tau}f_\sigma + \\ &\sum_\sigma \lambda_\sigma\left(f^\dagger_\sigma f_\sigma - p^\dagger_\sigma p_\sigma - d^\dagger d\right) + \sum_{k,\sigma} c^\dagger_{k,\sigma}\frac{d}{d\tau}c_{k,\sigma} + \\ &V\sum_{k,\sigma} c^\dagger_{k,\sigma} z_\sigma f_\sigma + h.c. + \sum(\epsilon_k-\mu)\,c^\dagger_k c_k + \\ &+\lambda_{KR}\left(e^\dagger e + \sum_\sigma p^\dagger_\sigma p_\sigma + d^\dagger d - 1\right) + \\ &+2\frac{V\bar{V}}{J} + \lambda_{SC}\left(e^\dagger e + d^\dagger d - K h^\dagger h\right). \end{aligned} \quad (23)$$

We find that the zero temperature meanfield partition function is given by:

$$\frac{1}{\beta}\ln(Z) = \frac{2}{\pi} Im\left[\xi \ln\left(\frac{\xi}{eD}\right)\right] - \frac{2\Delta}{\pi J\rho} - \sum_\sigma \lambda\left(p_\sigma^2 + d^2\right)$$
$$-\lambda_{SC}\left(d^2 + e^2 - K_1 h_1^\dagger h_1\right)$$
$$-\lambda_{KR}\left(\sum_\sigma p_\sigma^2 + d^2 + e^2 - 1\right) . \tag{24}$$

Here $\xi = iz^2\Delta + \lambda$ and $\lambda_\uparrow = \lambda_\downarrow = \lambda$. Furthermore,

$$z_\sigma = \left(1 - d^2 - p_\sigma^2\right)^{-\frac{1}{2}} 2d\left(p_\sigma + p_{-\sigma}\right)\left(1 - d^2 - p_{-\sigma}^2\right)^{-\frac{1}{2}}$$
$$= z_{-\sigma} \equiv z\,. \tag{25}$$

The self consistent mean field conditions (together with particle-hole symmetry) give us that

$$\frac{K}{2} = e^2 = d^2 \tag{26}$$
$$= \frac{4\frac{\Delta}{\pi\rho J} + \lambda_{SC} - \sqrt{\left(4\frac{\Delta}{\pi\rho J} + \lambda_{SC}\right)^2 - 8\lambda_{SC}\frac{\Delta}{\pi\rho J}}}{4\lambda_{SC}} .$$

We note that for large $\lambda_{SC} \to \infty$, $K, e^2, d^2 \to 0$ and indeed we obtain a good projection onto the spin 1/2 subspace.

We also get that

$$p_\uparrow = p_\downarrow\,, \qquad p^2 = \frac{1}{2} - d^2\,, \tag{27}$$

and z given by Eq. (25) can be further simplified to:

$$z = 4dp = -2\left(p-d\right)^2 + 2p^2 + 2d^2 = 1 - 2\left(p-d\right)^2 . \tag{28}$$

Finally, we obtain, $\lambda_\uparrow, \lambda_\downarrow$, $\lambda_{KR} = \frac{1+4d^2}{2d^2}\frac{\Delta}{\pi\rho J}$ and

$$\Delta = z^{-2} D \exp\left(-\frac{z^{-2}}{\rho J}\right) . \tag{29}$$

We have now obtained a family of mean field solutions as a function of the parameter K that we introduced in our approach. We can take advantage of this freedom for instance to best fit one of the known properties of the Kondo model, for instance $T_K = \sqrt{\rho J} D \exp\left(\frac{-1}{\rho J}\right)$, which we can do analytically perturbatively for small ρJ. We now use the identify $\Delta \sim T_k = \sqrt{\rho J} D \exp\left(\frac{-1}{\rho J}\right)$, $\rho J \ll 1$, then we get:

$$\exp\left(-\frac{z^{-2}}{\rho J}\right) \simeq \sqrt{\rho J}\exp\left(\frac{-1}{\rho J}\right) , \tag{30}$$

and

$$z^{-2} \simeq 1 - \frac{1}{2}\rho J \ln(\rho J)\,, \quad z \simeq 1 + \frac{1}{4}\rho J \ln(\rho J) . \tag{31}$$

We then get:

$$d^2 \simeq \frac{1}{4} - \frac{1}{32}\frac{\lambda_{SC}}{\frac{\Delta}{\pi\rho J}}, \quad 2\left(p-d\right)^2 \simeq \frac{1}{16}\left(\frac{\lambda_{SC}}{\frac{\Delta}{\pi\rho J}}\right)^2 . \tag{32}$$

This means that:

$$\left(\frac{\lambda_{SC}}{\frac{\Delta}{\pi\rho J}}\right)^2 = -4\rho J \ln(\rho J)\,, \quad \lambda_{SC} = \frac{2\Delta}{\pi}\sqrt{\frac{4\ln(1/\rho J)}{\rho J}} . \tag{33}$$

Once we have tuned K to match the Kondo temperature, we can obtain the heat capacity

$$C_v = 2k_B^2 T\frac{\pi^2}{3}\frac{1}{z^2\Delta}\left(-\ln z + 1\right) \simeq 2k_B^2 T\frac{\pi^2}{3}\frac{1}{z^2\Delta}\,, \tag{34}$$

and the magnetic susceptibility

$$\chi \simeq \frac{g^2\mu_B^2}{-\pi\lambda_{SC} z^{-2} + 2\pi p z^2\Delta + 3\lambda_{SC}}$$
$$\simeq \frac{g^2\mu_B^2}{2\pi p z^2\Delta_0} \simeq \frac{g^2\mu_B^2}{\pi\Delta} . \tag{35}$$

Correspondingly, the Wilson ratio is

$$w = \frac{2}{\pi} + ... \simeq 0.64\,, \tag{36}$$

which is also improved with respect to the conventional Read-Newns mean field value of one.

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