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X.Y. Zhang

and

G.M. Zhang

INTERNATIONAL ATOMIC ENERGY AGENCY

UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

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X.Y. Zhang and G.M. Zhang [1]
International Centre for Theoretical Physics, Trieste, Italy.

ABSTRACT

We present an asymptotically exact solution of the $\infty - d$ Hubbard model at a special interaction strength U_T corresponding to the strong-coupling Fermi-liquid fixed point. This solution is intimately related to the Toulouse limit of the single-impurity Kondo model and the symmetric Anderson model in its strong-coupling limit.

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[1]Permanent address: Pohl Institute of Solid State Physics, Tongji University, Shanghai 200092, People's Republic of China.

Introduction: Ever since the original introduction of the $\infty - d$ Hubbard model by Metzner and Vollhardt [1], and the recognition that the large-d limit model has a k-independent self-energy, the hope for an exact solution has been high. After a series of important analytical work [2]- [9], and the recent surge in numerical simulations of the model, some of the outstanding physical processes described by the model have been gradually made clear. [10]- [14]. Yet, any exact solution is still out of sight. The bottleneck is: although the k-independent self-energy $\Sigma(\omega)$ has reduced the problem to a $0+1$ dimensional one with a self-consistency, it is still highly non-trivial to calculate the Green's function of the corresponding "impurity" problem, which is crucial for the self-consistency to be complete.

Here, we present a solution which is exact in the asymptotic limit, *i.e.* $\tau \to \infty$. The solution is obtained only at half-filling with a special interaction U.

We first sketch the lines of reasoning reaching this solution: (i) The $\infty - d$ Hubbard model is mapped to a single impurity Anderson model with a self-consistent condition [8]. The condition requires loosely speaking, that the local Green's function to have the same form as its surrounding conduction electron bath characterized by a hybridization function. (ii) As the interaction U is increased, the dynamics of the impurity model is governed by the "Kondo" physics, where there is an asymptotic point, called the Toulouse limit (TL) [15], at which the problem is exactly soluble. It will be shown that the corresponding symmetric Anderson Model also possesses such a limit, where the asymptotic behavior of the local Green's function can be obtained. (iii) With this Green's function, the self-consistent procedure can be carried out. It is found that, at the TL, the asymptotic behavior of the impurity Green's function can be made consistent with that of the hybridization function, thus the $\infty - d$ Hubbard model is solved asymptotically.

Toulouse limit of the symmetric impurity Anderson model: It is well known that the single-impurity Kondo model has such an asymptotic limit: TL, where the conduction electrons become free [15], [16]. Similar limit exists for the Anderson model. We first remind the readers how this limit is derived for the Kondo model emphasizing on the concept rather than the details.

First, the Kondo Hamiltonian is separated into two parts, $H = H_0 + H_I$, where $H_0 = \sum_{k,\sigma}\epsilon_k C^\dagger_{k,\sigma}C_{k,\sigma} + \frac{J_z}{2}S_z\sum_{k,k'}(C^\dagger_{k,\uparrow}C_{k',\uparrow} - C^\dagger_{k,\downarrow}C_{k',\downarrow})$ and $H_I = J_\perp\sum_{k,k'}(S^+C^\dagger_{k,\downarrow}C_{k,\uparrow} + S^-C^\dagger_{k,\uparrow}C_{k,\downarrow})$. Because of the spin-flip term H_I, a given spin sector of the system, say, the up spin, constantly undergoes transition between the eigen states of $H_i = \sum_k \epsilon_k C^\dagger_{k,\uparrow}C_{k,\uparrow} + \frac{J_z}{4}\sum_{k,k'}C^\dagger_{k,\uparrow}C_{k',\uparrow}$, and that of $H_f = \sum_k \epsilon_k C^\dagger_{k,\uparrow}C_{k,\uparrow} - \frac{J_z}{4}\sum_{k,k'}C^\dagger_{k,\uparrow}C_{k',\uparrow}$. The two eigen states have a relative phase shift, $\delta = 2tan^{-1}\frac{\pi\rho J_z}{4}$, which is reflected in the propagator between the two states, $\langle|e^{iH_i t}C_\uparrow e^{-iH_f t}C^\dagger_\uparrow|\rangle \approx t^{-(1-\delta/\pi)^2}$. This is the origin of the non-Fermi liquid behavior of the X-ray edge problem [17], [18]. When the phase shift takes a particular value, such that the exponent in the asymptotic Green's function becomes $2(1-\frac{\delta}{\pi})^2 = 1$, or $\rho J_z = \frac{4}{\pi}ctg(\frac{\pi}{2\sqrt{2}})$, the Fermi-liquid (FL) behavior $\frac{1}{\tau}$ is restored [19], and the system appears to be free. This is the origin of the TL. The restoring of the FL behavior for an arbitrary phase shift δ is a much more subtle result first pointed out by Anderson *et al.* [16].

The symmetric Anderson model

$$H = \sum_{k,\sigma}\epsilon_k C^\dagger_{k,\sigma}C_{k,\sigma} + V\sum_{k,\sigma}(C^\dagger_{k,\sigma}f_\sigma + h.c.) + Un^f_\uparrow n^f_\downarrow - \frac{U}{2}(n^f_\uparrow + n^f_\downarrow), \tag{1}$$

does not have a spin-flip term explicitly. But via a discrete Hubbard-Stratonovich transformation [20], we can write the partition function as,

$$Z = \sum_{\{\sigma_l=\pm 1\}} Tr\left(e^{-\Delta\tau H(\sigma_1)}e^{-\Delta\tau H(\sigma_2)}.....e^{-\Delta\tau H(\sigma_L)}\right), \tag{2}$$

where $\frac{1}{2}\sum_\sigma e^{\lambda\sigma(n_\uparrow - n_\downarrow)} = e^{[-Un_\uparrow n_\downarrow + \frac{1}{2}(n_\uparrow + n_\downarrow)U]\Delta\tau}$ and $cosh\lambda = e^{(\frac{U}{2}\Delta\tau)}$. Just like in the Kondo model, for a given spin sector, say the up spin, the system is alternating between eigen states of $H_i = H_0 + \frac{\lambda}{\Delta\tau}f^\dagger_\uparrow f_\uparrow$ $(\sigma = 1)$ and that of $H_f = H_0 - \frac{\lambda}{\Delta\tau}f^\dagger_\uparrow f_\uparrow$ $(\sigma = -1)$. Here $H_0 = \sum_k \epsilon_k C^\dagger_{k,\uparrow}C_{k,\uparrow} + V\sum_k(C^\dagger_{k,\uparrow}f_\uparrow + f^\dagger_\uparrow C_{k,\uparrow})$. The phase shift of conduction electrons between these two eigen states is $\delta = 2tan^{-1}(\frac{\pi V^2\rho_f}{\frac{\lambda}{\Delta\tau}})$ [21].

For a given sequence of $\{\sigma_l\} = ++++----++++$, where the flips are taking place longer than the relaxation time [17], [16], [21], there is a well-defined phase shift between the flipped states and the unflipped ones. This is reflected in the evolution operator, $u(\tau) = \langle|e^{H_i\tau}e^{-H_f\tau}|\rangle$. The reason that it is an evolution operator instead of a Green's

function is because the spin-flip terms are absent here. This absence is compensated by the presence of the $f-$electrons in the Hamiltonian, which will contribute to an overall phase shift of π, so that $\langle u(\tau)u^\dagger(\tau')\rangle \approx (\tau-\tau')^{-(1-\frac{\delta}{\pi})^2}$ still holds.

To arrive at the TL point, the sum σ is first regrouped into sections that contain equal number of spin-flips, n. Within each section, the positions of the spin-flips are summed. $\sum_{\sigma_1\sigma_2\sigma_3...\sigma_L} = \sum_n\int\frac{d\tau_1}{\Delta\tau}\int\frac{d\tau_2}{\Delta\tau}.....$, and the average is written as an exponential, [18]

$$\langle u(\tau_1)u^\dagger(\tau_2)u(\tau_3)....u^\dagger(\tau_n)\rangle = e^{-(1-\frac{\delta}{\pi})^2\sum_{i>j}(-1)^{i+j}ln|\frac{\tau_i-\tau_j}{\Delta\tau}|}.$$

The partition function thus takes the form,

$$Z = \sum_{n=0}^{\infty}\int_0^\beta\frac{d\tau_{2n}}{\Delta\tau}\int_0^{\tau_{2n}-\Delta\tau}\frac{d\tau_{2n-1}}{\Delta\tau}...\int_0^{\tau_2-\Delta\tau}\frac{d\tau_1}{\Delta\tau}e^{-\left(2(1-\frac{\delta}{\pi})^2\sum_{i>j}(-1)^{i+j}ln|\frac{(\tau_i-\tau_j)}{\Delta\tau}|\right)}. \tag{3}$$

Once the TL is set, *i.e.* the coefficient in front of the logarithmic function becomes unity, the partition function is just the same as that of the following Hamiltonian:

$$H_T = \sum_k \epsilon_k C^\dagger_k C_k + V_T\sum_k(C^\dagger_k d + h.c.), \tag{4}$$

where V_T depends on the chemical potential of the Coulomb gas which is ignored so far, but will be introduced in the following calculations. Since H_T is free, the impurity Green's function $< d(t)d^\dagger(0) >$ can be easily obtained.

Notice that the same Coulomb gas formula (3) was derived long time ago by Hamann [21] in his path integral approach. His tunneling configurations are the domain walls of the Ising variables here. That the symmetric Anderson model also has a TL is not surprising, considering the fact that via Schrieffer-Wolff transformation one can map it into a Kondo model. The subtlety is, this transformation allows one to go to a weak-coupling J of the Kondo, whereas the TL is a strong-coupling limit. The fact that the low-energy physics in the weak-coupling limit is controlled by the strong-coupling fixed point, keeps the physics of TL alive.

Local Green's function of the symmetric impurity Anderson model: Comparing (1) to (4), the effect of the σ's sum is to push the effective f level to the Fermi point, *i.e.* zero, and

to renormalize the coupling parameters such that the low energy behavior of the f-electrons is replaced by that of spinless d-electrons. In fact, as pointed out by Anderson *et al.* [16], $\langle n^f(t)n^d(0)\rangle = \langle S_z(t)S_z(0)\rangle$. This leads to a natural intuitive identification of d with f [22]. One can express the low frequency part of the Green's function as:

$$\langle f(t)f^\dagger(0)\rangle_{low} \approx \frac{\Delta}{D}\langle d(t)d^\dagger(0)\rangle, \tag{5}$$

where Δ/D is the spectral weight of the low frequency part. The weight of the high frequency part can be well approximated once the system is in the strong coupling regime, and the bare band shape is known. The sum of the two is unity obeying the sum rule.

Another way of insuring the validity of the above relationship, is to use the slave-boson or slave-fermion decomposition scheme [23], to separate f-electrons as $f_\sigma = ab_\sigma + \sigma d^\dagger b^\dagger_{-\sigma}$. To constrain the f's in a singly occupied state, we restrict the bosons to $\sum_\sigma b^\dagger_\sigma b_\sigma = 1$. It is then straight forwardly shown that $S_z = \frac{1}{2}(b^\dagger_\uparrow b_\uparrow - b^\dagger_\downarrow b_\downarrow) = b^\dagger_\uparrow b_\uparrow - 1/2, S^\dagger = b^\dagger_\uparrow b_\downarrow, S^- = b^\dagger_\downarrow b_\uparrow$, the usual Schwinger boson representation of the spin operators. If we neglect the doublon part, then we have $< f_\uparrow(t)f^\dagger_\uparrow(0) >= \langle a(t)a^\dagger(0)b_\uparrow(t)b^\dagger_\uparrow(0)\rangle \approx \langle a(t)a^\dagger(0)\rangle\langle b_\uparrow(t)b^\dagger_\uparrow(0)\rangle \propto \langle b_\uparrow(t)b^\dagger_\uparrow(0)\rangle$, where one particle per site constraint has been enforced. On the other hand, we can write $< d(t)d^\dagger(0) >=< S^-(t)S^+(0) >$ using the spinless fermion representation of the local spin operator. We then replace the spin operator by Schwinger bosons, such that, $\langle d(t)d^\dagger(0)\rangle =< b^\dagger_\downarrow(t)b_\uparrow(t)b^\dagger_\uparrow(0)b_\downarrow(0) >\approx< b_\uparrow(t)b^\dagger_\uparrow(0) >$. Thus, we obtain eq.(5).

An exact asymptotic solution of the $\infty - d$ Hubbard model: As pointed out by Georges and Kotliar [8], the most fruitful way to make use of a site-independent self-energy is to map the model to an Anderson impurity model plus a self-consistency. The impurity Lagrangian,

$$\pounds = -\int\int d\tau d\tau' C^\dagger_\sigma G_0^{-1} C_\sigma + \int d\tau U(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2}), \tag{6}$$

where G_0 is the Green's function with site 0, "the impurity site" removed. One first calculates G from $\pounds$, and relates G to G_0 by, $G^{-1}(\omega) = G_0^{-1}(\omega) - \Sigma(\omega)$, thereby closing up the self-consistency. On a Bethe lattice, this relation is simplified to $G_0^{-1} = z - t^2 G$. The asymptotic form of G_0 can be obtained from its spectral density representation, $G_0(\tau) = \int_0^\infty \rho_0(\epsilon)e^{-\epsilon\tau}d\epsilon$.

At zero temperature, $G_0(\tau) = \frac{\rho_0(0)}{\tau} + O(\frac{1}{\tau^2})$. For $\infty - d$ Hubbard model, $\rho_0(0)$ is pinned [2], because $\Sigma(0) = 0$, so that $G(0) = G_0(0)$. On a Bethe lattice, the value of the pinning is $\frac{2}{\pi D}$, where D is the radius of the semi-circle density of states.

If we represent G_0 in terms of "integrated" conduction electrons in the Anderson Model, as we are allowed to do in the case of Bethe lattice, $G_0^{-1} = z - V^2\Sigma\frac{1}{z-\epsilon_k}$, we can transform (6) to (1) with a conduction electron density of states to be self-consistently determined. In this way, simply borrowing the last section can give the TL for the large-d Hubbard model. But here, we would like to derive this asymptotic limit in the Lagrangian formulation. The final results are the same.

The partition function of the effective impurity version of the $\infty - d$ Hubbard model can be written as

$$Z = \sum_{\{\sigma_i=\pm 1\}} det(G_0^{-1} + \frac{\lambda}{\Delta\tau}\sigma)det(G_0^{-1} - \frac{\lambda}{\Delta\tau}\sigma), \tag{7}$$

where the same discrete Hubbard-Stratonovich transformation is used. To obtain the Coulomb gas form, we make the following expansions of the determinants:

$$det\hat{O}_\sigma det\hat{O}_{-\sigma} = e^{-Tr(G_0\frac{\lambda}{\Delta\tau}\sigma)^2 + TrO(G_0^4)\cdots}, \tag{8}$$

where $\hat{O}_\sigma = I + G_0\frac{\lambda}{\Delta\tau}\sigma$. Since $G_0 \to \frac{2}{\pi D}\frac{1}{\tau}$, it is enough to keep only the second order part to obtain the asymptotic limit. Taking the trace in the imaginary time, $Tr(G_0\sigma)^2 = \int d\tau_1 \int d\tau_2 G_0(\tau_1 - \tau_2)\sigma(\tau_2)G_0(\tau_2 - \tau_1)\sigma(\tau_1)$ and using the fact $G_0(\tau) = -G_0(-\tau)$, we have

$$Z = e^{2(\frac{2\lambda}{\pi D\Delta\tau})^2 \sum_{i>j}\sigma_i\frac{1}{(i-j)^2}\sigma_j + \mu\sigma_i\sigma_{i+1}}, \tag{9}$$

where μ is the chemical potential governed by the short time behavior of G_0 to be determined below. This long range 1-d Ising model can be mapped to a Coulomb gas model [16], [24]. The interaction strength in front of the logarithmics is $2(\frac{2\lambda}{\pi D\Delta\tau})^2$. When this is set to unity, we obtain the TL of the $\infty - d$ Hubbard model: $\sqrt{\frac{U}{\Delta\tau}} = \frac{\pi D}{2\sqrt{2}}$, where we have approximated $\lambda \approx \sqrt{U\Delta\tau}$. The low frequency part of the Green's function can be obtained from (4) (5):

$$G(\omega)_{low} = \frac{\Delta/D}{\omega - V_T{}^2\Sigma_k\frac{1}{\omega-\epsilon_k}} \approx \frac{\Delta/D}{\omega + i\Gamma} \tag{10}$$

where $V_T = \frac{e^{-\mu}}{\Delta\tau}$, and $\Gamma \equiv \pi V_T^2 \rho(0) = \frac{2}{D} V_T^2$. Since $G(0) = \frac{2}{iD}$, we have $\Delta = \frac{4}{D\Delta\tau^2} e^{-2\mu}$, from which Δ can be determined, because μ is a function of Δ.

Although the asymptotic solution $G(\tau) = \frac{2}{\pi D}\frac{1}{\tau}$ does not depend on Δ, neither does U_T, it is essential that Δ being finite [25] for the TL to exist as can be seen from eq.(10). To determine Δ, we have to consider the short time behavior or high energy part of G_0 which is lattice dependent and cannot be calculated accurately within this framework. Fortunately, at least for the Bethe lattice, we can obtain an approximate value of Δ, which is finite at U_T, and thus proving the existence of the TL.

At zero temperature, and for $\tau > 0$, $G_0(\tau) = \int_0^\infty \rho_0(\epsilon) e^{-\epsilon\tau} d\epsilon$ where $\rho_0 = -\frac{1}{\pi} Im G_0$. The TL point is a strong coupling point. Our numerical experience with the Bethe lattice in this region shows that ρ_0 consists of a $\delta-$like peak around $z_0 = \sqrt{\Delta D}$ in addition to the finite part $\frac{2}{\pi D}$ at $z = 0$. The former contributes to the short time behavior of $G_0(\tau)$, the latter to the long time behavior. This has been derived analytically in Ref. [26]. For completeness, we rederive it briefly here. On the Bethe lattice, $G_0 = \frac{1}{z - t^2 G}$. The G can be decomposed into a sum of low and high energy parts, $G = G_{low} + G_{high}$. Here G_{low} is the one obtained from eq.(4) and G_{high} can be written as $\int \frac{\rho_h(\epsilon) d\epsilon}{\omega - \epsilon}$ where ρ_h only counts for the high energy part so that $\rho_h(\epsilon \to 0) \to 0$. For a small Δ, in the region $\Delta < z < \sqrt{\Delta D}$, $G_{high}(z) \approx -z \int \frac{\rho_h(\epsilon) d\epsilon}{\epsilon^2}$, and $G_{low}(z) \approx \frac{\Delta/D}{z}$. Thus, we have $G_0(z) \approx \frac{z}{z^2(1+C) - t^2\Delta/D}$ where $C = t^2 \int \frac{\rho_h d\epsilon}{\epsilon^2}$ and $t = D/2$. The position of the δ-like peak is found at, $z_0 = \frac{1}{2}(\frac{\Delta D}{1+C})^{\frac{1}{2}}$ with a weight of $\frac{1}{2(1+C)}$. So, for τ being finite, we have: $G_0(\tau) \approx \frac{1}{2(1+C)} e^{-z_0\tau}$. Using (8) and (9), we obtain the chemical potential from the short time part of G_0: $\mu \approx \frac{\lambda^2}{4(1+C)^2} e^{-2z_0\Delta\tau}$.

So far, everything is dependent on the cut-off $\Delta\tau$. There are certain arbitrariness in choosing this cut-off, which will affect the exact values of U_T and Δ. This is deeply rooted in the TL of the impurity models. Fortunately, the main result of this paper, *i.e.* the form of the asymptotic solution and the existence of this solution is independent of the choice of the cut-off. We adapt Hamann's choice of the cut-off $\Delta\tau = \frac{6}{U}$ [21]. With this choice and an estimate of $C \approx t^2/(\frac{u}{2})^2 = (\frac{D}{U_T})^2$, we have, $U_T = 2.6D$ and $\Delta = 0.2D$. The result is

very close to the second order perturbation calculation [11], although as we pointed out, the exact number comparison is not very meaningful due to the cut-off dependence.

For a hypercubic lattice, the kinetic energy is more spread out because of the Gaussian density of states in contrast to the semi-circular one. As a result, for the same value of interaction U, Δ is expected to be larger. Therefore, the TL will also exist there although the calculation in determine Δ is much more complicated.

Discussion: (i) We want to emphasize that the TL point obtained from the Coulomb gas analogy is valid only asymptotically. In the Bethe Ansatz solution of the Anderson impurity model, there is no special value of U at which the rapidity equation becomes free. The same can be said about the Kondo model: even though there is a TL-like limit in the Bethe ansatz solution, it is different from the one derived by Toulouse [15] or Anderson *et al.* [16]. The difference lies in the phase shift. The Toulouse line in the Bethe ansatz solution intersects with the Wilson fixed point [22]. The phase shift of the Wilson fixed point is π, the well-known unitary limit. The phase shift of the TL point is $(1 - \frac{\sqrt{2}}{2})\pi$, and is independent of the $J_\perp$. In this sense, the usual TL does not show up in the Bethe ansatz for the Kondo problem either.

(ii) The approximation involved here is to assume certain path being important, *i.e.* the spin-flips are separated long enough so that the system has a chance to relax. In this way, the concept of phase shift can be used. In the Kondo regime, the interval of the adjacent spin-flip is about the order of the inverse Kondo temperature, which is long compare to the relaxation time. Therefore, this approximation becomes exact in the asymptotic sense.

(iii) Within the above mentioned limitations, we have derived an exact asymptotic point of the $\infty - d$ Hubbard model, which corresponds to the strong-coupling FL fixed point. The form of the solution itself does not provide any new information about the model. This is due to a special feature of the large-d limit: the density of states is pinned on the metallic side. As long as the FL assumption is correct, one can arrive at this solution [8]. But, the FL assumption can and does break down when the interaction strength is large enough [10]. The assumption has to be self-consistent to be valid. As stated in the beginning, this is the

most difficult part of the $\infty - d$ Hubbard model. The contribution of this work is to show how the self-consistency can be achieved exactly at one point. To generalize to arbitrary interaction strength, we have also tried and failed to use another asymptotic approaches for this problem, namely, the conformal field theory [27].

(iv) A more fruitful way of using the TL is to go away from half-filling, where much less has been understood. All the derivations used here are applicable except for one: the distinction between the high energy part and the low energy part spectral weight becomes blurred, thus making it more difficult to determine the value of Δ.

(v) Through out the derivations, we have emphasized on the phase shift. Once the phase shift takes a special value, the model appears to be free. In this sense, X-ray edge problem also has a TL [28], where the Anderson catastrophe seemingly goes away. But unlike the X-ray edge problem where the phase shift is well-defined between given initial and final states, for the single-impurity models and the $\infty - d$ Hubbard model, the phase shift is only meaningful in an intermediate step of a special treatment: the path-integral approach. In this special language, the system is phase-shifting back and forth until it is equilibrated. As creatively conjectured by Anderson *et al.* [16], no matter what the phase shift is, as the system equilibrates, it will only take one value, the TL. This one statement turns out to involve all the machinery of many-body physics to justify and to modify [29]. Thus, the essence of solving the model at the TL directly is to reach the strong coupling point without encountering the formidable task. The present work is just one more example in exploiting this limit [30].

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