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On the functional integral approach in quantum statistics: I. Some approximations

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Abstract. In this paper the susceptibility of a Kondo system in a fairly wide temperature region is calculated in the first-harmonic approximation in a functional integral approach. The comparison with the value obtained by renormalization group theory shows that in this region the two results agree quite well. The expansion of the partition function with infinite independent harmonics for the Anderson model is studied. Some symmetry relations are generalized. It is a challenging problem to develop a functional integral approach including diagram analysis, mixed-mode effects and some exact relations in the Anderson system proved in a functional integral approach. These topics will be discussed in a subsequent paper.

1. Introduction

There has been much interest recently in the valence fluctuation phenomena which are observed in some metallic rare-earth compounds [1, 2]. The 4f level of the rare-earth ions may be shifted from magnetic to non-magnetic behaviour under hydrostatic pressure. At high temperatures the magnetic susceptibility contains a fraction of the Curie susceptibility. At low temperatures no magnetic ordering has been observed and the susceptibility tends to be constant. In view of a number of measurements [1, 2], it is now apparent that rare-earth ions, e.g. Sm and Ce, have mixed valence states, which consist of a magnetic and a non-magnetic configuration. Several theoretical models have been proposed to describe such a phenomenon [3].

The asymmetric Anderson model gives, in principle, a valid description of a dilute fluctuating-valence system. A Hartree–Fock approximation or mean-field theory has been used to study this model [4–6]. Krishna-Murthy *et al* [7] have applied the renormalization group approach to study the single-impurity asymmetric Anderson model. Their numerical results on the impurity susceptibility in their well-known papers [7] show that this model shares many features of the magnetic susceptibilities in mixed-valence compounds. The present author and Ting [8] have studied the same problem with the functional integral approach (FIA). Using number theory and cancelling the singularities in the integrands, the susceptibility in a fairly wide range of temperatures can be calculated and the results agree quite well with those of the renormalization group calculation of Krishna-Murthy *et al* for ε_l, the f level lying above the Fermi level.

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Furthermore we also calculate the f-electron occupation number $\bar{n}_l$ as a function of temperature and the f-electron energy level, the results show that $\bar{n}_l$ depends on $\mathscr{E}_l$ when $\mathscr{E}_l$ is close to the Fermi level. Then one can give a physical explanation for the fluctuating-valence phenomenon.

The symmetric Anderson model can also be used to study the Kondo effect [4, 7, 9] and the problem related to magnetic impurities in metals. Although the Anderson model and the Kondo problem have been excellently studied by the renormalization group approach [7] and the Bethe *ansatz* [10, 11], it is still interesting to develop the study of the FIA further. Because a theorem in section 2 shows that a fairly general class of problems in quantum statistics can be formulated by the FIA, it has a sound foundation and a hopeful future. From a practical point of view, it can give an exact formal solution for the Anderson model and can realize a suitable concrete calculation [8, 12, 14–16]. Some difficulties have been overcome continuously. In section 2 a functional integral formulation for the general problem in quantum statistics and some numerical calculations in the first order harmonic approximation (FHA) for the Anderson model are reviewed. In section 3 an expansion with infinite independent harmonics is studied. Some numerical results from the FIA are obtained for the Kondo system and compared with those from the renormalization group approach. In a subsequent paper we shall discuss the theoretical framework of the FIA without divergence, the Feynman diagram analysis in the FIA with complex representation, and some exact relations in the Anderson system proved by the FIA. The concluding remarks are given in section 4.

2. Functional integral formulation in quantum statistics

It is interesting to transform quantum statistical problems into ideal gas problems by the FIA.

Theorem. A general statistical equilibrium problem can be transformed into a problem of an ideal gas moving in a (complex) time-dependent external field. The price that one needs to pay is introducing a functional integral.

Proof. It is obvious the Hamiltonian of many-body systems with potential interaction can be written as

$$\hat{H} = \hat{H}'_0 + \hat{H}'_{\text{int}} \tag{2.1}$$

where

$$\hat{H}'_{\text{int}} = \frac{1}{2V}\sum_q \sum_{k\sigma} \sum_{k'\sigma'} U(q)\hat{a}^+_{k'+q,\sigma'}\hat{a}^+_{k-q,\sigma}\hat{a}_{k\sigma}\hat{a}_{k'\sigma'}. \tag{2.2}$$

$$\hat{H}'_0 = \sum_{kk'\sigma} (I_{kk'} + \tfrac{1}{2}U_0\delta_{kk'}]\hat{a}^+_{k\sigma}\hat{a}_{k'\sigma} \tag{2.3}$$

and U_0 is the potential at the origin.

$$\hat{H}'_{\text{int}} = \sum_q \hat{A}_q\hat{B}_q$$

where

$$\hat{A}_q = \hat{B}_q = \sum_{k\sigma} \sqrt{\frac{U(q)}{2V}}\, \hat{a}^+_{k+q,\sigma}\hat{a}_{k\sigma}. \tag{2.4}$$

Let us follow the well-known works [14–18]. Introduce

$$\begin{aligned} A^\mu_q &= \int_0^\beta \exp(\mathrm{i}\Omega_\mu \tau)\, \hat{A}_q(\tau)\, \mathrm{d}\tau \qquad \beta = (kT)^{-1} \\ B^\mu_q &= \int_0^\beta \exp(\mathrm{i}\Omega_\mu \tau)\, \hat{B}_q(\tau)\, \mathrm{d}\tau \qquad \Omega_\mu = \frac{2\pi}{\beta}\mu \end{aligned} \tag{2.5}$$

and the Feynman–Dyson expansion. Noticing that A^μ_q, B^μ_q and $\hat{H}_0$ commute under the time-ordering operator T and the Stratonovich–Hubbard [17, 18] identity is still valid even when $\hat{A}_q$ and $\hat{B}_q$ are not Hermitian, we obtain for the expression of partition function

$$\begin{aligned} \Xi = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_q \prod_{\mu=-\infty}^{\infty} \mathrm{d}x^\mu_q\, \mathrm{d}y^\mu_q \exp(-\pi |z^\mu_q|^2) \\ \times \mathrm{Tr}\Big[\exp(-\beta\hat{H}_0)\, \hat{T} \exp\Big(-\sqrt{\frac{\pi}{\beta}} \sum_q \sum_\mu A^\mu_q z^{-\mu}_q - B^\mu_q (z^{-\mu}_q)^*\Big)\Big] \end{aligned} \tag{2.6}$$

where

$$z^\mu_q = x^\mu_q + \mathrm{i}y^\mu_q. \tag{2.7}$$

Letting

$$z_q(\tau) = \sum_{\mu=-\infty}^{\infty} z^\mu_q \exp(-\mathrm{i}\Omega_\mu \tau) \tag{2.8}$$

and transforming (2.6) into the time representation, we have

$$\Xi = \int \mathrm{D}z \exp\Big(-\frac{\pi}{\beta}\int_0^\beta \sum_q |z_q(\tau)|^2\Big)\, \Xi_1(z) \tag{2.9}$$

where

$$\Xi_\lambda(z) = \mathrm{Tr}\Big[\hat{T}\exp\Big(-\int_0^\beta \hat{H}_\lambda(\tau)\, \mathrm{d}\tau\Big)\Big] \tag{2.10}$$

$$\hat{H}_\lambda(\tau) = \hat{H}_0 + \lambda \sum_q C_q(\tau) \sum_{k\sigma} \hat{a}^+_{k+q,\sigma}(\tau)\hat{a}_{k\sigma}(\tau) \tag{2.11}$$

$$C_q(\tau) = \sqrt{\pi/2\beta V}\,[\sqrt{U(q)}\, z_q(\tau) - \sqrt{U(-q)}\, z^*_{-q}(\tau)] \tag{2.12}$$

$$\mathrm{D}z = \prod_q \prod_{\mu=-\infty}^{\infty} \mathrm{d}x^\mu_q\, \mathrm{d}y^\mu_q. \tag{2.13}$$

Equations (2.9) and (2.10) contain the theorem. The derivative of $\ln \Xi_\lambda$ with respect to λ can be expressed as follows:

$$\begin{aligned} \frac{\partial(\ln \Xi_\lambda)}{\partial\lambda} &= -\sum_q \int_0^\beta \frac{C_q(\tau)}{\Xi_\lambda}\, \mathrm{d}\tau\, \mathrm{Tr}\Big[\hat{T}\exp\Big(-\int_0^\beta \hat{H}_\lambda(\tau')\, \mathrm{d}\tau'\Big) \sum_{k\sigma} \hat{a}^+_{k+q,\sigma}(\tau)\hat{a}_{k\sigma}(\tau)\Big] \\ &= -\sum_q \int_0^\beta C_q(\tau)\, \mathrm{d}\tau \Big\langle \sum_{k\sigma} a^+_{k+q,\sigma}(\tau) a_{k\sigma}(\tau)\Big\rangle. \end{aligned} \tag{2.14}$$

Here $\langle \ldots \rangle$ means the average being taken over an ensemble with the Hamiltonian $\hat{H}_\lambda$ and can be obtained by the Green function theory. The definition of the temperature Green function of the operators $\hat{A}$ and $\hat{B}$ in the generalized Heisenberg picture is

$$\langle\langle \hat{A}(\tau)\hat{B}(\tau')\rangle\rangle = \mathrm{Tr}[\hat{\rho}_\lambda \hat{T}\hat{A}(\tau)\hat{B}(\tau')] \tag{2.15}$$

where

$$\tilde{O}(\tau) = s^{-1}(\tau)\hat{O}s(\tau); s(\tau) = \hat{T}\exp\left(-\int_0^\tau \hat{H}_\lambda(\tau')\,\mathrm{d}\tau'\right) \tag{2.16}$$

and the density matrix is given by

$$\hat{\rho} = s(\beta)/\Xi_\lambda. \tag{2.17}$$

As an important example, one can consider the Anderson model:

$$\hat{H} = \sum_{k\sigma} \varepsilon_{k\sigma}\hat{n}_{k\sigma} + \sum_{\sigma} \varepsilon_{l\sigma}\hat{n}_{l\sigma} + \sum_{k\sigma}(V_{kl}\hat{a}^+_{k\sigma}\hat{b}_{l\sigma} + \mathrm{cc}) + \hat{H}_{\mathrm{int}}$$

$$\hat{H}_{\mathrm{int}} = U\hat{n}_{l\uparrow}\hat{n}_{l\downarrow}. \tag{2.18}$$

In this case, if we introduce U_0 and q, $\hat{A}_q(\tau)$ and $\hat{B}_q(\tau)$ in equation (2.5) are replaced by $\sqrt{U}\hat{n}_{l\uparrow}$ and $\sqrt{U}\hat{n}_{l\downarrow}$, respectively. The corresponding problem of an ideal gas in a complex external field can be solved exactly [12] and the formal solution of the partition function Ξ is obtained [12, 16]

$$\Xi = \Xi_{U=0}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\left(\prod_{\mu=-\infty}^{\infty}\mathrm{d}x_\mu\,\mathrm{d}y_\mu\exp(-\pi|z_\mu|^2)\right)$$
$$\times\exp\left(\sum_\sigma \mathrm{Tr}[\ln(I-\hat{V}^\sigma G^{0\sigma}_{ll})\hat{A}]\right) \tag{2.19}$$

where

$$\begin{aligned}
&(\hat{A})_{nm} = \exp(\mathrm{i}\omega_n 0^+)\,\delta_{nm}\\
&(\hat{V}^\sigma)_{nm} = \beta C^\sigma_{n-m}\\
&C^\sigma(\tau) = \sqrt{u\pi/\beta}[\sigma x(\tau) + \mathrm{i}y(\tau)]\\
&(G^{0\sigma}_{ll})_{nm} = (\delta_{nm}/\beta)[\mathrm{i}\omega_n - \varepsilon_{l\sigma} - \Sigma_n]^{-1}\\
&\Sigma_n = -\mathrm{i}\overline{|V|^2}N(0)\sin(\omega_n)\\
&\Gamma = \pi\overline{|V|^2}N(0) \qquad \delta = \beta\Gamma/\pi
\end{aligned} \tag{2.20}$$

where $N(0)$ and $\overline{|V^2|}$ are the density of states and the average of the interaction matrix element square at the Fermi surface and Γ is the width of the f level.

$$\Xi_{U=0} = \mathrm{Tr}[\exp(-\beta\hat{H}_0)]$$
$$= \Xi_{\mathrm{band}}\exp\left[-\sum_\sigma\frac{\beta\varepsilon_{l\sigma}}{2} - \ln(2\pi) + 2\ln\left|\Gamma\left(\frac{1}{2}+\frac{\delta}{2}+\mathrm{i}\frac{\beta\varepsilon_{l\sigma}}{2\pi}\right)\right|\right].$$

In studies of the FIA, many well-known physicists have made great contributions to studies of the Anderson system. In 1965, Mühlschlegel [14] pointed out that the generalized Hartree–Fock approximation (i.e. the static approximation) can be obtained by only keeping $\mu = 0$ and is exact in high-temperature region or for $V \to 0$. Wang *et al*

[15] discussed the FHA and RPA′ in the real representation; Hamann [12] gave the formal solution (2.19). The complex representation of the FIA was developed by Mühlschlegel [14], Hamann [12] and Amit and Keiter [16]. The superiorities of complex representation was emphasized by Amit and Keiter [16]. In particular, for a zero magnetic field and the symmetric Anderson model, the partition function maintains the following symmetry relation:

$$\Xi(U) = \exp(\beta U/2)\,\Xi(-U) \tag{2.21}$$

which is easily overlooked in the approximation to a real representation [16]. In addition, the FHA is studied and some numerical calculations of susceptibility in the high-temperature range for the symmetric case are given in the FHA. In our paper [8], we have applied the FIA to discuss the susceptibility χ and the f-electron occupation number for the asymmetric case and to obtain the following symmetry relations, for all U and T:

$$\chi(X_0) = \chi(1 - X_0) \qquad X_0 = -\varepsilon_l/U \tag{2.22}$$

$$\bar{n}_l(1 - X_0) = 2 - \bar{n}_l(X_0). \tag{2.23}$$

Equation (2.22) is consistent with that of the renormalization group approach; equation (2.23) is new. Overcoming a series of difficulties, introducing an integration method in number theory and cancelling the divergence of integrands at the boundaries, χ and $\bar{n}_l$ for the asymmetric Anderson system have been calculated in a fairly wide temperature range and compared with that of the renormalization group approach.

In order to separate the static approximation from other effects, let

$$\hat{V}^\sigma = \hat{V}_0^\sigma + \tilde{V}^\sigma \tag{2.24}$$

where

$$\hat{V}_0^\sigma = (\hat{V}^\sigma)_{nn}\delta_{nn'} \qquad (\tilde{V}^\sigma)_{nn'} = \hat{V}^\sigma_{nn'}(1 - \delta_{nn'}). \tag{2.25}$$

One obtains [16]

$$\begin{aligned}\Xi = f\int_{-\infty}^{\infty} \mathrm{d}(\mathrm{Re}\,\bar{z}_0)\int_{-\infty}^{\infty}\mathrm{d}(\mathrm{Im}\,\bar{z}_0)\exp(-\pi|\bar{z}_0|^2)\\ \times\prod_\sigma[\Gamma(1+A^\sigma)\Gamma(1+B^\sigma)]^{-1}\left(\prod_{\mu\neq 0}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}x_\mu\,\mathrm{d}y_\mu\exp(-\pi|z_\mu|^2)\right)\\ \times\exp\left(\sum_\sigma \mathrm{Tr}[\ln(\hat{I} - \tilde{V}^\sigma\tilde{G}_0^\sigma)]\right)\end{aligned} \tag{2.26}$$

where

$$\begin{pmatrix}A^\sigma\\ B^\sigma\end{pmatrix} = (\delta - 1)/2 \mp (1/2\pi\mathrm{i})(\beta\bar{\varepsilon}_{l\sigma} - \bar{V}_0^\sigma) \qquad \bar{\varepsilon}_{l\sigma} = \bar{\varepsilon}_{l\sigma} + U/2. \tag{2.27}$$

$$(\tilde{G}_0^\sigma)_{nn'} = (\delta_{nn'}/2\pi\mathrm{i})\begin{cases}1/(n+1+A^\sigma) & (n \geqslant 0)\\ 1/(n-B^\sigma) & (n \leqslant -1)\end{cases} \tag{2.28}$$

$$f = \Xi_{\mathrm{band}}(2\pi)^2\exp[-(\beta/2)(\bar{\varepsilon}_{l\uparrow} + \bar{\varepsilon}_{l\downarrow} - U/2] \tag{2.29}$$

$$\bar{V}_0^\sigma = \sqrt{\pi\beta U}(\sigma\bar{x}_0 + i\bar{y}_0). \tag{2.30}$$

Denoting

$$\hat{Q}^\sigma \equiv \hat{I} - \bar{V}^\sigma \tilde{G}_0^\sigma \tag{2.31}$$

in the FHA, only terms with $\mu = 0, \pm 1$ are considered:

$$\exp\left(\sum_\sigma \mathrm{Tr}(\ln \hat{Q}^\sigma)\right) \simeq \det[D_1^\sigma] \tag{2.32}$$

where

$$(D_1^\sigma)_{mn} = \begin{cases} 1 & m = n \\ -\bar{V}_\nu^\sigma \tilde{G}_0^\sigma(n) & m = n + \nu \\ -\bar{V}_{-\nu}^\sigma \tilde{G}_0^\sigma(n) & m = n - \nu \\ 0 & \text{otherwise} \end{cases} \tag{2.33}$$

and $\det(D_1^\sigma)$ can be calculated by the Bessel function theory [16, 19]. In this approximation the susceptibility χ and occupation number $\bar{n}_f$ of f electrons are expressed by [16]

$$\chi = (\beta/4)(g\mu_B)^2\langle(x_1 - x_2)^2\rangle \tag{2.34}$$

$$\bar{n}_f = 2 - \langle(x_1 + x_2)\rangle \tag{2.35}$$

where

$$\langle A\rangle \equiv \frac{1}{\bar{\Xi}}\int_0^1\int_0^1 \mathrm{d}x_1\,\mathrm{d}x_2\,\bar{\Xi}(x_1, x_2)A \tag{2.36}$$

$$\bar{\Xi} \equiv \int_0^1\int_0^1 \mathrm{d}x_1\,\mathrm{d}x_2\,\bar{\Xi}(x_1, x_2) \tag{2.37}$$

$$\bar{\Xi}(x_1, x_2) = \sum_{m=0}^{\infty} \frac{(Y_0\delta)^{2m}}{\Gamma^2(m + 1 + \delta)} 4^{\delta-1}[\sin(\pi x_1)\sin(\pi x_2)]^{\delta+2m-1}$$
$$\times \exp\{\pi^2 Y_0\delta[(\tfrac{1}{2} - X_0)(x_1 + x_2 - 1) - (x_1 - \tfrac{1}{2})(x_2 - \tfrac{1}{2})]\}$$
$$Y_0 = U/\pi\Gamma \qquad X_0 = -\varepsilon_f/U. \tag{2.38}$$

Some misprints in these formulae in [8] have been corrected.

In the fluctuating-valence problem, Y_0 is very large (possibly 10^2), the integrands vary rapidly and change in the range of $\exp(\pm 100)$, and the coefficients in equation (2.38) change in the range of $\exp(\pm 180)$. The double integrals and the sum in equation (2.38) converge very slowly. One meets a series of serious difficulties and much computing time is needed. We have adopted a powerful multidimensional integration method developed by Hua and Wang [20] on the basis of number theory which overcomes a series of difficulties. In a rather wide temperature range we calculate the susceptibility χ and compare it with that of the renormalization group theory in [7]. For example, some comparisons are shown in figures 4–8 of [8]. Moreover, we also calculate the plots of $\bar{n}_f$ as a function of $X_0 = -\varepsilon_f/U$. These relations show that $\bar{n}_f$ changes rapidly in the vicinities of $X_0 = 0$ or 1. So it is also explained why the number of valence electrons is an integer in the usual cases.

3. Expansion with infinite independent harmonics and numerical results for the Kondo system

One of the important topics in [16] is the superiority of complex representation in the FIA. In particular, it maintains the symmetry relation (2.21) in the FHA. We have proved the symmetry relations (2.22) and (2.23). In this section we shall discuss their validity in higher-order approximations.

An infinite independent harmonic approximation means that, in the expansion (2.26), only the terms with Z_ν and $Z_{-\nu}$ are considered and all the other terms with a mixed mode, e.g. $Z_{\nu_1}, z_{\nu_2}, z_{-\nu_1-\nu_2}, \ldots$ are neglected. This corresponds to the following approximation, suggested in [16]:

$$\exp[\mathrm{Tr}(\ln Q^\sigma)] \simeq 1 + \sum_{\nu=1}^{\infty} [\det(D_1^\sigma) - 1]. \tag{3.1}$$

Using the recursion relation for $\det(D_\nu^\sigma)$, we obtain

$$\det(D_\nu^\sigma) = \prod_{k=0}^{\nu-1} \left(\frac{\delta}{\nu}\right) \Gamma\left[\frac{1}{\nu}(A^\sigma + 1 + K)\right] \Gamma\left[\frac{1}{\nu}(B^\sigma + \nu - k)\right] \sum_{m_k=0}^{\infty} \frac{1}{m_k!}$$
$$\times \frac{(-1)^{m_k}[\bar{v}_\nu^\sigma \bar{v}_{-\nu}^\sigma/(2\pi i\nu)^2]^{m_k} \Gamma[\delta/\nu + 2m_k]}{\Gamma[m_k + (1/\nu)(A^\sigma + 1 + k)]\Gamma[m_k + (1/\nu)(B^\sigma + \nu - k)]\Gamma[\delta/\nu + m_k + 1]}. \tag{3.2}$$

Substituting (3.2) into (3.1) and (2.26), after some lengthy calculations and carrying out all the infinite dimensional integral except $\nu = 0$, we obtain the formula for the partition function Ξ, according to the following formulae:

$$\chi = kT\,\partial^2 \ln \Xi / \partial \mathcal{H}^2 - \chi_{\text{band}} \tag{3.3}$$

$$\bar{n}_l = -kT \sum_\sigma \frac{\delta(\ln \Xi)}{\delta \varepsilon_{l\sigma}}. \tag{3.4}$$

We obtain the expressions for the susceptibility χ and occupation number $\bar{n}_l$ for f electrons. In order to save space, we omit the details and write the resultant expressions directly:

$$\chi = \frac{1}{\Xi} \sum_{\nu=1}^{\infty} \frac{(g\mu_B)^2}{4\nu^2 kT} \int_{-1/2}^{1/2} \cdots \int_{-1/2}^{1/2} \sum_{k=0}^{\nu-1} (\zeta_k - \eta_k)^2 \Xi_\nu \prod_{k=0}^{\nu-1} \mathrm{d}\zeta_k\, \mathrm{d}\eta_k \tag{3.5}$$

$$\bar{n}_l = 1 + \frac{1}{\Xi} \sum_{\nu=1}^{\infty} \int_{-1/2}^{1/2} \cdots \int_{-1/2}^{1/2} \frac{1}{\nu} \sum_{k=0}^{\nu-1} (\zeta_k + \eta_k) \Xi_\nu \prod_{k=0}^{\nu-1} \mathrm{d}\zeta_k\, \mathrm{d}\eta_k \tag{3.6}$$

where

$$\Xi = \sum_{\nu=1}^{\infty} \int_{-1/2}^{1/2} \cdots \int_{-1/2}^{1/2} \Xi_\nu \prod_{k=0}^{\nu-1} \mathrm{d}\zeta_k\, \mathrm{d}\eta_k \tag{3.7}$$

$$\Xi_\nu = f \sum_{\{m_k\}} \sum_{\{m'_{k'}\}} \left(\frac{\beta U}{4\pi^2\nu^2}\right)^{2m} \Gamma^2(m+1)\delta_{mm'}(2\pi)^{2\nu-2}\nu^{-2\delta}\left(\frac{\delta}{\nu}\right)^{2\nu}$$
$$\times \prod_{k=0}^{\nu-1} \prod_{k'=0}^{\nu-1} \frac{[2\cos(\pi\zeta_k)]^{2m_k+\delta/\nu-1}[2\cos(\pi\eta_k)]^{2m'_{k'}+\delta/\nu-1}}{m_k!\Gamma[\delta/\nu + m_k + 1]m'_{k'}!\Gamma[\delta/\nu + m'_{k'} + 1]}$$

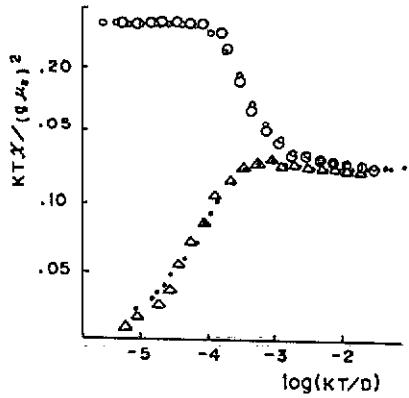

Figure 1. Semilogarithmic plots of $kT\chi/(g\mu_B)^2$ versus kT/D for the symmetric Anderson model for $Y_0 = 12.665$ (○, ○) and $Y_0 = 1.0132$ (△, ●): ○, △, results for [7]; ○, ●, results of FIA.

$$\times \exp\left(\frac{\mathrm{i}}{\nu}\sum_{k=0}^{\nu-1}(1+2k-\nu)\pi\zeta_k + \frac{\mathrm{i}}{\nu}\sum_{k=0}^{\nu-1}(1+2k'-\nu)\pi\eta_k\right)$$

$$\times \exp\left(-\frac{1}{\nu}\beta\bar{\varepsilon}_{l\uparrow}\sum_{k=0}^{\nu-1}\zeta_k - \frac{1}{\nu}\beta\bar{\varepsilon}_{l\downarrow}\sum_{k=0}^{\nu-1}\eta_k - \frac{\beta U}{2}\sum_{k=0}^{\nu-1}\zeta_k\sum_{k=0}^{\nu-1}\eta_k\right) \tag{3.8}$$

for $\qquad m = \sum_{k=0}^{\nu-1} m_k \geqslant 1 - \delta_{\nu,1}.$

According to equations (3.5)–(3.8), we conclude the following.

(i) The static approximation [14] and the FHA [8, 16] are special cases corresponding to $\nu = 0$ and $\nu = 0.1$, respectively.

(ii) For all T and Y_0, Ξ_ν has the following symmetry relations:

$$\Xi_\nu(X_0, Y_0, \{\zeta_k\}, \{\eta_k\}) = \Xi_\nu(X_0, Y_0, \{\eta_k\}, \{\zeta_k\}) \qquad \text{when } H = 0 \tag{3.9a}$$

$$\Xi_\nu(1 - X_0, Y_0, \{\zeta_k\}, \{\eta_k\}) = \Xi_\nu^*(X_0, Y_0, \{-\zeta_k\}, \{-\eta_k\}) \qquad \text{for all } H. \tag{3.9b}$$

Here one can see that in the complex representation it is easy to lose reality but we can prove in general that in this kind of problem the imaginary parts of Ξ must be zero. Then we have

$$\Xi_\nu(1 - X_0, Y_0, \{\zeta_k\}, \{\eta_k\}) = \Xi_\nu(X_0, Y_0, \{-\zeta_k\}, \{-\eta_k\}). \tag{3.10}$$

According to equations (3.5)–(3.10), we can prove the following properties.

In the infinite independent harmonic approximation, for all temperatures T and Coulomb energy U, Anderson systems possess the following symmetry properties:

$$\bar{n}_l(Y_0, X_0 = 0.5) = 1 \tag{3.11}$$

$$\chi(Y_0, 1 - X_0) = \chi(Y_0, X_0) \tag{3.12}$$

$$\bar{n}_l(Y_0, 1 - X_0) = 2 - \bar{n}_l(Y_0, X_0). \tag{3.13}$$

The property in (3.11) has been proved previously only in mean-field theory [21, 22].

The property in (3.12) is inconsistent with that of the renormalization group approach [7]. The property in (3.13) is new. These identities are valid not only in the FHA but also in the infinite independent harmonic approximation.

Now let us consider the Kondo system, or the symmetric Anderson model, which is one of the important cases. Krishna-Murthy *et al* [7] studied it excellently with the renormalization group approach. Amit and Keiter [16] studied the same problem by FIA in the high-temperature region. Because the temperature region is too narrow ($\delta \simeq$ 0–6), the susceptibility curve corresponds to the horizontal part in figure 1 and cannot display the curved part: so the comparison between two approaches cannot be realized.

We try to make a serious comparison between the two approaches in the symmetric Anderson system and need to perform a calculation of the susceptibility over a fairly wide temperature region ($\delta \simeq 0$–10^3). Then we meet with many serious difficulties.

(a) The integrands change very rapidly and on a large scale. When the variable changes from 0 to 1, sometimes the integrands change from $\exp(-10^5)$ to $\exp(10^5)$. The way in which these integrands can be handled and use them in a computer is a rather difficult problem.

(b) When δ is very large, the series converges very slowly. Sometimes one needs thousands of terms with double integrals. Much computing time is necessary.

(c) When δ is very large, a large number of coefficients need to be calculated. It is well known that in ordinary computers, for example, $\Gamma^2(25)$ will overflow but, for $Y_0 = 12$, one needs $\Gamma^2(1000)$ and large $(Y_0\delta)^{2m}$. We have met the first of these difficulties already in the fluctuating-valence problem [8]. The second and third are new.

After making great efforts for a long time, including introducing the integration method based on number theory [20] and other measures, we have overcome all these difficulties and performed the calculation of the susceptibility for f electrons in a fairly wide temperature region. Both the numerical results of [7] and ours are demonstrated in figure 1. The comparison shows that in this fairly wide temperature region our results by the FIA agree quite well with those of Krishna-Murthy *et al* [7] obtained by the renormalization group approach.

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