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On the functional-integral approach in quantum statistics, including mixed-mode effects and free of divergences: II. Diagram analysis and some exact relations

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Abstract. In this paper the causes of the 'mathematical breakdown' of the random-phase approximation RPA' are analysed. Starting from an exact matrix formula, a diagram analysis of a functional-integral approach is developed with the following characteristics: (i) All the singularities of the integrands are cancelled completely; there is no problem of the limitation from the convergence radius of the formula used. (ii) The reality of the partition functions at every stage is guaranteed and all the benefits of the complex representation are preserved simultaneously. (iii) All the functional-integral series are transformed into two-dimensional integral series. (iv) A functional-integral approach, which can calculate the mixed mode contributions, is given for the first time. The diagrammatic rules of mixed mode contributions and some concrete examples are given. Some exact symmetry relations and expressions are suggested and proved. These symmetry relations are also preserved at every stage in our diagram analysis. They are useful in practical calculations. A new exact relation is also derived.

1. Introduction

This series is devoted to studying the functional-integral approach (FIA) in quantum statistics. In the first paper [1], a theorem shows that 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 one needs to pay is introducing a functional integral. The susceptibility of a Kondo system in a fairly wide temperature region is calculated in the first harmonic approximation (FHA) in the FIA. The comparison with that of renormalization group theory (RGT) shows that in this region these two results agree quite well. The expansion of the partition function with infinite independent harmonics for the Anderson model is studied and used to discuss some symmetry relations. The occupation number and susceptibility of asymmetric Anderson systems are studied by FIA in [2], and their results are compared with that of renormalization group theory in [3].

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It is well known that there is a 'mathematical breakdown' in the famous random-phase approximation (RPA′) of the FIA. Amit and Keiter [4] neglect all the mixed mode effects and suggest the independent harmonic approximation to avoid this difficulty. But the divergence problem still needs to be solved. This paper is devoted to developing a systematic diagram analysis of the FIA, including the mixed mode effects and free of divergences.

In section 2, the cause of the 'mathematical breakdown' of RPA′ is investigated. The validity of a useful formula is analysed.

In section 3, a systematic diagram analysis of an expansion of the partition function in the FIA is given. The cancellation theorem of divergence is proved. All the singularities of the integrands are cancelled in every order. The reality theorem is proved. Then the reality of the partition function in every order is guaranteed even in the complex representation of FIA.

In section 4, the contributions from mixed modes are included in the theoretical framework in a natural way. The diagrammatic rules of mixed mode contributions and some concrete examples, especially the lowest-order (third-order) mixed mode contributions, are calculated.

In section 5, as applications of the diagram analysis, some exact symmetry relations and expressions for Anderson systems are proved. They are useful in practical calculations. Some symmetry relations, which are pointed out and proved in the independent harmonic approximations in [2] and [1], are proved to be exact.

In section 6, the same topics as in section 5 are discussed for Anderson systems with attractive Coulomb interactions (negative U).

The concluding remarks and discussions are given in section 7.

2. The cause of RPA′ divergence in FIA and a matrix formula

It is interesting to introduce a Feynman diagram analysis in the FIA, because the diagrams may be useful in discussing the following problems:

(i) How to make a systematic expansion that is exact and allows for further approximations beyond the independent harmonic approximation or RPA′.

(ii) What will happen at very low temperature in the symmetric case.

(iii) The difference of the results of renormalization group approach and FIA when the f level is below the Fermi level.

This is not an easy task.

Keiter [6] has discussed the Anderson model from the viewpoint of a diagrammatic perturbation technique in the real representation. One of the remarkable achievements is that the author establishes the relation between the FIA and the perturbation expansions by means of comparison. But some questions still exist. For example, these approaches, including RPA′, are based on an elementary formula:

$$\ln(1+x) = -\sum_{m=1}^{\infty} \frac{(-x)^m}{m} \qquad (-1 < x \leq 1). \tag{2.1}$$

But in these approaches in the vicinities of the singularities of the Green function, x turns to infinity. In principle, expansion (2.1) is no longer valid when $|x| > 1$. We have no reason to believe that the integrations from $-\infty$ to $+\infty$ are still correct.

As pointed out by Amit and Keiter [4], in the higher-order RPA' [5] one faces higher order pole singularities and some terms in the expansions are divergent. Then they neglect all the mixed mode effects, suggest the independent harmonic approximation to avoid this difficulty. (But the mixed mode effects have not been included yet.) It is a challenging problem to build in the mixed mode contributions to the theory. It is also interesting to eliminate the divergence of all the diagrams at the beginning. So a systematic analysis of the expansion in the FIA is still needed.

In order to establish a systematic diagram analysis of FIA, including the mixed mode effects and free of divergences, instead of formula (2.1), we start from the formula

$$\exp(\mathrm{Tr}\ln A) = \det(\hat{A}) \tag{2.2}$$

which can be proved in the following cases:

(i) When $\hat{A}$ is Hermitian. Formula (2.2) can be proved easily in the eigen-representation. Please note that here $\hat{A}$ can be an infinite-dimensional matrix and its eigenvalues can be any real number.

(ii) When $\hat{A}$ is not Hermitian and

$$|\lambda_{nn} - 1| < 1. \tag{2.3}$$

Formula (2.2) can be proved in the linear operator theory [7] starting from (2.1) for an $N \times N$ matrix, the infinite determinant follows then in the limit $N \to \infty$ as in [4].

(iii) When $\hat{A}$ is not Hermitian and

$$|\lambda_{nn} - 1| > 1. \tag{2.4}$$

Then formula (2.1) is no longer valid. The main point of this discussion is to emphasize the subtle difference of the validity conditions of the formulae (2.1) and (2.2).

For a logarithmic function $\ln(z)$, the only singularity in the finite region is the branch point at $z = 0$. Usually, in order to make the function single-valued, one uses a branch cut starting at $z = 0$, or fix on the leaf of the Riemann surface. But analytic continuation between two leaves of the Riemann surface is still available. Following [8], one can change the expansion centre, using analytic continuation to avoid the singularity. According to the Abel theorem and choosing a suitable expansion centre A_0, we always have

$$\ln\hat{A} = \sum_{m=0}^{\infty} C_m(\hat{A}_0 - A_0)^m \tag{2.5}$$

where

$$|A_{nn} - A_0| < r \qquad C_m(A_0) = (\mathrm{d}^m/\mathrm{d}A_0^m)\ln(A_0)/m! \tag{2.6}$$

and r is the convergence radius. One can also use the similarity transformation to get the same expression (2.5).

Not all the linear operators can be diagonalized by a non-singular transformation even for a finite matrix, but all the matrices can be transformed into subdiagonal form by a unitary transformation [7]. According to the properties of subdiagonal matrices, we have

$$\mathrm{Tr}\ln\hat{A} = \sum_n \sum_{m=0}^{\infty} C_m(A_0)(A_{nn} - A_0)^m = \sum_n \ln(A_{nn}). \tag{2.7}$$

Formula (2.2) is valid and independent of the magnitudes of the eigenvalues and the expansion forms, even in the cases in which formula (2.1) does not exist. The formula (2.2) is proved.

Usually infinite matrices can be considered as the limiting case. For Hermitian matrices, the formula is proved even in infinite matrices. For infinite non-Hermitian matrices, if when $N \to \infty$, the limit of the RHS of expression (2.7) exists and is finite, then formula (2.2) is still valid. As to a discussion on the more general condition from a mathematical viewpoint, we shall leave this as an interesting open problem.

The main point is that in the FIA, x denotes a function of the Green functions. In the vicinities of singularities of Green functions, x turns to infinity continuously. Certainly one can use the expression (2.5) or

$$\ln \hat{A} = \ln A_0 - \sum_{m=1}^{\infty} \frac{1}{m}\left(1 - \frac{\hat{A}}{A_0}\right)^m . \tag{2.8}$$

Although (2.5) or (2.8) can be derived from (2.1) by transformation, they are eventually different from (2.1). In the usual theory of FIA, one always neglects this difference. In the integration one uses expression (2.1) only and errors are built in to the theory at the beginning. Even if one notices this difference and uses (2.5) or (2.8), one cannot change A_0 continuously in a practical calculation of the functional integral, because that is too complicated. The merit of formula (2.2) is that the form of the formula is unified and independent of the magnitude of the eigenvalues of $\hat{A}$. This merit is important for our following study in the theoretical framework of the FIA.

3. Feynman diagram analysis in the functional-integral approach, including mixed mode effects and free of divergences

In this section the first problem is how to establish a systematic expansion in the FIA without divergence and develop a corresponding Feynman-diagram analysis. The second problem is how to maintain all the benefits of the complex representation and guarantee the reality of the partition function in every order simultaneously. The third problem is how to transfer all the functional integrals corresponding to the expansion diagrams into finite-dimensional integrals. The fourth problem is how to include the coherent effect of mixed modes. Up to now one has still needed a FIA including mixed mode effects in a natural way. Surely they are important at low temperature. This problem is a challenging one. We try to establish a systematic approach in FIA by solving these problems.

3.1. Theoretical expansion in FIA and cancellation theorem of divergence

Hereafter the symbols used follow [1]. As pointed out by Amit and Keiter [4], there is a 'mathematical breakdown' in the famous RPA' in FIA [5]. The generalized RPA' [4] consists of two steps: expanding the logarithmic operator according to (2.1); admitting the index in the matrix elements to have only the values $\pm\nu$ [4]. Then

$$\exp\left(\sum_{\sigma} \operatorname{Tr}\ln(I - \tilde{V}^{\sigma}\tilde{G}_0^{\sigma})\right) \simeq \prod_{\sigma}\prod_{\nu>0} \det(D_{\nu}^{\sigma}). \tag{3.1}$$

Some spurious terms enter into the expansion, when $\nu \geqslant 2$; the pole singularities of higher order lead to divergence.

It is worth noting that in the vicinities of the singularities of $\hat{Q}^\sigma$, the expansion (2.1) is no longer valid owing to the finite convergence radius and divergence occurs. Because the RPA' is a selective partial summation of expansion (2.1), we assert that the main danger comes from expansion (2.1).

It is also worth noting that the divergence is only a signal: even in the finite region $|x| > 1$, expansion (2.1) already loses its meaning. The road leading out of the dilemma is to avoid expansion (2.1).

Fortunately we can use an exact linear operator identity as the starting point:

$$\exp(\mathrm{Tr}\ln \hat{A}) = \det(\hat{A}). \tag{3.2}$$

This formula transforms the combinational operation with logarithm into a determinant and is independent of the magnitudes of the eigenvalues. Certainly if one makes an incorrect approximation in the determinant, one can still get a divergent result.

To avoid superpositions of poles, we expand the determinant exactly according to the definition of the determinant. Then establishing the exact diagram rules, we can develop a natural diagram analysis.

It is obvious that

$$\exp\left(\sum_\sigma \mathrm{Tr}\ln \hat{Q}^\sigma\right) = \prod_\sigma \det(\hat{Q}^\sigma). \tag{3.3}$$

Consider the infinite matrix Q^σ as a limit of the corresponding $2m \times 2m$ matrix with $m \to \infty$. Its centre is close to Q^σ_{00}; the position of the centre is $(-0.5, -0.5)$. Introduce g^σ_0, q^σ and new label n:

$$g^\sigma_0(n) \equiv \tilde{G}^\sigma_0(n-m-1) \qquad n = 1, 2, \ldots, 2m \tag{3.4}$$

$$q^\sigma_{nn} \equiv Q^\sigma_{n-m-1,n'-m-1} = \begin{cases} 1 & \text{if } n = n' \\ -\bar{v}^\sigma_{nn'} g^\sigma_0(n') & \text{otherwise.} \end{cases} \tag{3.5}$$

The merits of this procedure will be explained later. We call this kind of section a 'mirror symmetric section'.

According to the definition of determinant we have

$$\det(Q^\sigma) = \sum_p (-1)^p q^\sigma_{1\alpha_1} q^\sigma_{2\alpha_2} \cdots q^\sigma_{2m,\alpha_{2m}} \tag{3.6}$$

where p is the inverse number of the permutation:

$$\begin{pmatrix} 1, & 2, & 3, & \ldots, & 2m \\ \alpha_1, & \alpha_2, & \alpha_3, & \ldots, & \alpha_{2m} \end{pmatrix}. \tag{3.7}$$

A cancellation theorem of divergence. In the expansion (2.26) in [1], all the singularities of the integrands in every term are removable.

Proof. In the expansion of $\det(Q^\sigma)$, only one term equals 1, and all others contain one or more factors for $\tilde{G}^\sigma_0$, possessing isolated singularities at the following points, according to (2.28) in [1]:

$$\begin{aligned} 1 + A^\sigma &= 0, -1, -2, \ldots \\ 1 + B^\sigma &= 0, -1, -2, \ldots. \end{aligned} \tag{3.8}$$

Because of the property of determinants, all the arguments in g^σ_0 in a term of expansion (3.6) are different and all the singularities in the expansion are simple poles.

Fortunately, there is a factor $[\Pi_\sigma \Gamma(1 + A^\sigma)\Gamma(1 + B^\sigma)]^{-1}$ in expansion (2.26) in [1], which possesses infinite simple zeros exactly at the same points (3.8). Just these simple zeros cancel all the possible singularities in the expansion of $\det(Q^\sigma)$ and all singularities in the integrands become removable.

Because of Gaussian factors, all the integrals in the expansion are convergent. This allows us to establish diagram rules and a systematic diagrammatic analysis.

Theorem. All the terms in the expansion (2.26) in [1] can be traced to double integrals.

Proof. Consider a general term containing $m_0\ q^{\uparrow}_{nn} = 1$ and $m'_0\ q^{\downarrow}_{nn} = 1$ and expressed by

$$u_k = (-1)^{p+p'-m_0}(U\beta\pi)^{M-(m_0+m'_0)/2} g(\boldsymbol{\alpha}, \boldsymbol{\beta}) z_{-M+1}^{k_{-M+1}} \dots z_{M-1}^{k_{M-1}} z_{-M+1}^{*k'_{-M+1}} \dots z_{M-1}^{*k'_{M-1}} \tag{3.9}$$

where

$$M = 2m \qquad \boldsymbol{\alpha} \equiv (\alpha_1, \alpha_2, \dots, \alpha_M) \qquad \boldsymbol{\beta} \equiv (\beta_1, \beta_2, \dots, \beta_M)$$

$$g(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \prod_{j=1}^{M} [g_0^g(\alpha_j)]^{a_j} [g_0^g(\beta_j)]^{b_j} \tag{3.10}$$

$$a_j = 1 - \delta_{j,\alpha_j} \qquad b_j = 1 - \delta_{j,\beta_j}.$$

Because $g(\boldsymbol{\alpha}, \boldsymbol{\beta})$ depends on z_0, z_0^* only, all the Gaussian integrations over z_μ and z_μ^* (except $\mu = 0$) can be carried out by the following orthogonal formula:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp(-\pi |z_\mu|^2) z_\mu^{k_\mu} z_\mu^{*k'_\mu}\, \mathrm{d}x_\mu\, \mathrm{d}y_\mu = \frac{k_\mu!}{\pi^{k_\mu}} \delta_{k_\mu, k'_\mu}. \tag{3.11}$$

We obtain

$$\Xi = f \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp(-\pi |\bar{z}_0|^2)\, \mathrm{d}\bar{x}_0\, \mathrm{d}\bar{y}_0 \left(\sum_k \bar{u}_k \right) \left(\prod_\sigma \Gamma(1 + A^\sigma)\Gamma(1 + B^\sigma) \right)^{-1} \tag{3.12}$$

$$\bar{u}_k = (-1)^{p+p'-m_0}(U\beta\pi)^{M-m_0} g(\boldsymbol{\alpha}, \boldsymbol{\beta}) \delta(k - k') \prod_{\mu=1-2m}^{2m-1} \left(\frac{k_\mu!}{\pi^{k_\mu}} \right) \tag{3.13}$$

where

$$k \equiv (k_{-2m+1}, \dots, k_{2m-1}) \qquad k' \equiv (k'_{-2m+1}, \dots, k'_{2m-1}). \tag{3.14}$$

We have now finished the transformation from the functional-integral expansion to a series of double integrals.

3.2. *Diagram rules*

In order to analyse the expansion systematically, we introduce a special diagram analysis. Following Feynman's idea on the diagram technique, we establish the correspondence between terms and diagrams.

The prescription for drawing a diagram of u_k is as follows:

(i) Set three rows of $2m$ equidistant points. The labels in the upper, middle and lower rows are integer sequences $\{n'\}$, $\{n_0\}$, $\{n\}$, respectively. The sequence $\{n_0\}$ has natural order. The permutation

$$\binom{\{n_0\}}{\{n\}}$$

corresponds to that of a term in $\det(Q^{\uparrow})$. The permutation

$$\binom{\{n_0\}}{\{n'\}}$$

corresponds to that of a term in $\det(Q^{\downarrow})$.

(ii) For $\sigma = \downarrow$ ($\sigma = \uparrow$), an arrow starting from point n_0 in the middle row pointing to point n' in the upper row (point n in the lower row) corresponds to $z^*_{n_0-n'}$ (z_{n_0-n}) respectively. Their physical explanation can be the amplitudes of fluctuations in complex fields with frequencies $\omega_{n_0-n'}$ (ω_{n_0-n}) in the mean-field background.

The prescription for writing down the contribution of $\bar{u}_k$ corresponding to a given diagram is the following:

(i) According to the configuration of arrows, check the factor $\Pi_\mu\, z_\mu^{k_\mu}\, z_\mu^{*k'_\mu}$ first:

$$\begin{aligned} \bar{u}_k &= 0 \qquad \text{if}\,\{k_\mu \neq k'_\mu\} \\ \bar{u}_k &\neq 0 \qquad \text{if}\,\{k_\mu = k'_\mu\}. \end{aligned} \tag{3.15}$$

(ii) Determine the number of cross points for lower (upper) arrows, which equals the inverse number p (p'). Determine the number of lower arrows $l = 2m - m_0$. Multiply the integrand by a factor $(-1)^{p+p'+l}$.

(iii) For every lower (upper) arrow introduce a factor $\sqrt{(U\beta\pi)}\tilde{G}_0^{\uparrow}(n-m-1)$ ($\sqrt{(U\beta\pi)}\tilde{G}_0^{\downarrow}(n-m-1)$) into the integrand respectively.

(iv) Every factor $|z|^{2k_\mu}$ in the u_k corresponds to a factor $k_\mu!/\pi^{k_\mu}$ in the $\bar{u}_k$.

According to this prescription one can give expressions like (3.13).

3.3. Reality theorem

The reality of the partition function is a necessary condition in physics. But the complex auxiliary field $z(\tau)$ is introduced in the present FIA. It is easy to lose reality in some approximations. For example in the infinite independent harmonic approximation the Ξ_ν in equation (3.8) in [1] may be complex. So it is very important to guarantee the reality of the partition function in every approximation order. Modern studies on multiple series point out that the approximation mode is very important. In the limiting process one has many choices. The main problem is in what kind of section can reality be guaranteed in every step. After careful consideration and exploration, considering the character of $\hat{Q}^\sigma$, we found the mirror symmetric sections, defined in equations (3.4) and (3.5), are available.

Reality theorem. Under the mirror symmetric section, all the terms in expansion (3.12) are real.

Let us first introduce some concepts; the self-dual and dual diagrams:

(i) In the mirror symmetric section, the mid-perpendicular of n_0 axes divides the unlabelled diagram into two parts. In general these two parts are asymmetric. If the

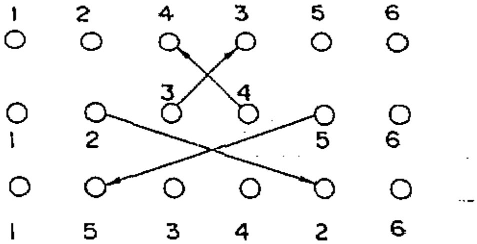

Figure 1. A typical self-dual diagram.

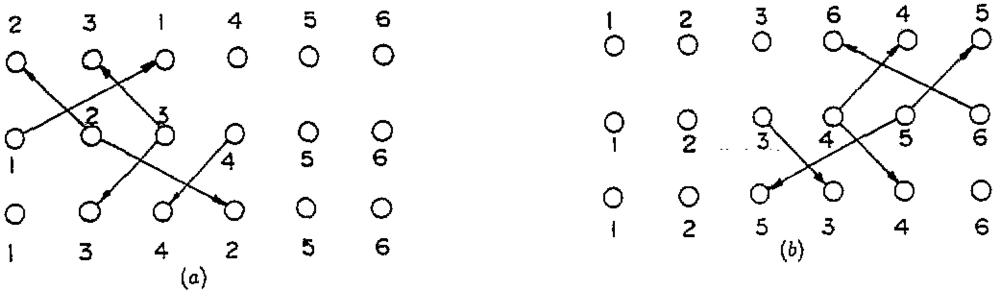

Figure 2. Two dual diagrams.

unlabelled diagram is mirror symmetric with respect to the mid-perpendicular, we call the diagram *self-dual.*

(ii) If an unlabelled diagram d is a mirror image of another diagram d′ with respect to the mid-perpendicular, we call then *dual* diagrams of each other.

For example, the diagram in figure 1 is self-dual and the diagrams in figure 2(a) and (b) are dual. It is obvious that in the mirror section all the diagrams must be either self-dual or dual.

Lemma 1. The contribution of every self-dual diagram is real.

Proof. Noticing that under mirror symmetric section in the self-dual diagram the factors of the Green function appear pairwise

$$\frac{-1}{(A^\sigma + \nu)(B^\sigma + \nu)} \tag{3.16}$$

the contribution of self-dual diagram u_k can be written as

$$\bar{u}_k(\mathrm{sd}) = \prod_\sigma f\left[\left\{\frac{1}{A^\sigma + \nu} \cdot \frac{-1}{B^\sigma + \nu}\right\}\right] [\Gamma(1 + A^\sigma)\Gamma(1 + B^\sigma)]^{-1}$$
$$\equiv \prod_\sigma F_\sigma(A^\sigma, B^\sigma) = \prod_\sigma F_\sigma(B^\sigma, A^\sigma). \tag{3.17}$$

Let

$$A^\sigma = \xi + \mathrm{i}b_\sigma - ay_0 + \mathrm{i}\sigma a x_0 \tag{3.18}$$

then

$$B^\sigma = \xi - \mathrm{i}b_\sigma + ay_0 - \mathrm{i}\sigma a x_0 \tag{3.18'}$$

where

$$\xi = (\delta - 1)/2 \qquad b_\sigma = (1/2\pi)\bar{\varepsilon}_{l\sigma}\beta \qquad a = (1/2\pi)\sqrt{(U\beta\pi)}. \tag{3.19}$$

We can prove that:

$$\begin{aligned}\langle u_k(\mathrm{sd})\rangle &\equiv \int_{-\infty}^{\infty} \mathrm{d}x_0 \int_{-\infty}^{\infty} \mathrm{d}y_0 \exp[-\pi(x_0^2 + y_0^2)]\bar{u}_k(\mathrm{sd}) \\ &= 2\int_{-\infty}^{\infty} \mathrm{d}x_0 \int_{0}^{\infty} \mathrm{d}y_0 \exp[-\pi(x_0^2 + y_0^2)] \\ &\quad \times \operatorname{Re} \prod_\sigma F_\sigma[\xi + \mathrm{i}b_\sigma - ay_0 + \mathrm{i}\sigma a x_0; \xi - \mathrm{i}b_\sigma + ay_0 - \mathrm{i}\sigma a x_0].\end{aligned} \tag{3.20}$$

Lemma 2. The resulting contribution of any pair of dual diagrams is real.

Proof. Suppose that the contribution of a diagram d can be expressed by $\bar{u}_k(\mathrm{d})$ as

$$\bar{u}_k(\mathrm{d}) = \prod_\sigma F_\sigma(A^\sigma, B^\sigma). \tag{3.21}$$

According to the properties of the Green function and the mirror symmetric section, the contribution of its dual diagram d′ is

$$\bar{u}_k(\mathrm{d}') = \prod_\sigma F_\sigma(B^\sigma, A^\sigma). \tag{3.22}$$

Suppose the contributions $\langle u_k(\mathrm{d})\rangle$ and $\langle u_k(\mathrm{d}')\rangle$, respectively, are not real. We can show that the resulting contribution must be real:

$$\begin{aligned}\langle \bar{u}_k(\mathrm{d}) + \bar{u}_k(\mathrm{d}')\rangle &= \int_{-\infty}^{\infty} \mathrm{d}x_0 \int_{-\infty}^{\infty} \mathrm{d}y_0 \exp(-\pi|z_0|^2) \\ &\quad \times \left(\prod_\sigma F_\sigma(A^\sigma, B^\sigma) + \prod_\sigma F_\sigma(B^\sigma, A^\sigma)\right) \\ &= 2\int_{-\infty}^{\infty} \mathrm{d}x_0 \int_{-\infty}^{\infty} \mathrm{d}y_0 \exp(-\pi|z_0|^2) \operatorname{Re}\left(\prod_\sigma F_\sigma(A^\sigma, B^\sigma)\right) \\ &= 2\operatorname{Re}\left\langle \prod_\sigma F_\sigma(A^\sigma, B^\sigma)\right\rangle.\end{aligned} \tag{3.23}$$

Combining lemmas 1 and 2, the reality theorem is valid under mirror symmetric section for finite matrix $\hat{Q}^\sigma$. It is obvious that the contributions of the diagrams are convergent. Then the results are limiting-mode independent. The reality theorem is proved.

4. Partial summations and diagrams with mixed modes

Now let us discuss the calculation of diagrams by the diagram analysis developed above. First of all classify the diagrams according to the arrow number l. We shall be concerned with the expansion in the low-temperature region.

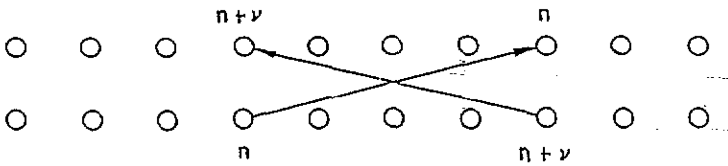

Figure 3. A typical diagram of second order.

(i) Zeroth order, $l = 0$. We have

$$g[0] = 1. \tag{4.1}$$

This is the static approximation.

(ii) First order, $l = 1$. According to the diagram analysis developed above, these kinds of diagrams will not appear:

$$g[\nu] = 0. \tag{4.2}$$

(iii) Second order, $l = 2$. Here

$$\begin{aligned} &g[\nu_1, \nu_2] = 0 \qquad (\nu_1 \neq -\nu_2) \\ &g[\nu_1, \nu_2] \neq 0 \qquad (\nu_1 = -\nu_2). \end{aligned} \tag{4.3}$$

The second-order diagrams exist only when $\nu_1 = -\nu_2$.

(iv) Third order, $l = 3$. These diagrams are different from the first one. The third-order diagrams do exist, for example $g[1,1,-2]$, $g[2,-1,-1]$, etc. In general the following diagram exists:

$$g[\nu_1, \nu_2, -(\nu_1 + \nu_2)]. \tag{4.4}$$

These are the lowest-order diagrams with mixed modes.

(v) Fourth order, $l = 4$. In this case

$g[\nu_1, -\nu_1], g[\nu_2, -\nu_2] \ldots$ are independent harmonic contributions

$g[\nu_1, \nu_2, \nu_3, -\nu_1 - \nu_2 - \nu_3]$ are mixed mode contributions.

(vi) Higher order: the contributions of these diagrams may be deduced by analogy.

Now let us discuss the second-order diagram shown in figure 3, which is a typical diagram of second order.

Partial summation is one of the important steps in the diagram technique: choose a class of diagrams and then sum them up. Summing over all the diagrams of second order with definite ν but different n, we obtain

$$\begin{aligned} g^\sigma[\nu, -\nu] &= -\bar{v}^\sigma_\nu \bar{v}^\sigma_{-\nu} \sum_{n=-\infty}^{\infty} \tilde{G}^\sigma_0(n) \tilde{G}^\sigma_0(n+\nu) \\ &= -(\bar{v}^\sigma_\nu \bar{v}^\sigma_{-\nu}/(2\pi \mathrm{i})^2) I^\sigma[\nu, -\nu]. \end{aligned} \tag{4.5}$$

Noting that

$$I^\sigma_1[\nu, -\nu] = \sum_{n=0}^{\infty} \frac{1}{(n+1+A^\sigma)(n+1+\nu+A^\sigma)} = \frac{1}{\nu} \sum_{k=0}^{\nu-1} \frac{1}{1+A^\sigma+k}$$

$$I^\sigma_2[\nu, -\nu] = \sum_{n=-\nu}^{-1} \frac{1}{(n-B^\sigma)(n+\nu+A^\sigma)} = \frac{1}{\nu+\delta} \sum_{n=1}^{\nu} \left(\frac{1}{n-\nu-1-A^\sigma} - \frac{1}{n-B^\sigma} \right)$$

$$I_3^\sigma[\nu, -\nu] = \sum_{n=-\infty}^{-\nu-1} \left(\frac{1}{(n-B^\sigma)(n+\nu-B^\sigma)}\right) = \frac{1}{\nu}\sum_{k=0}^{\nu-1} \frac{1}{1+B^\sigma+k}$$

we obtain

$$I^\sigma[\nu, -\nu] = \frac{1}{\nu}\sum_{k=0}^{\nu-1}\left(\frac{1}{1+A^\sigma+k} + \frac{1}{1+B^\sigma+k}\right)$$
$$+ \frac{1}{\delta+\nu}\sum_{n=1}^{\nu}\left(\frac{1}{n-\nu-1-A^\sigma} - \frac{1}{n-B^\sigma}\right). \tag{4.6}$$

Summing over all ν and taking the Gaussian average over all $\{z_\mu\}$, with $\nu \neq 0$, we obtain the exact contribution of all second-order diagrams, including all n and $\nu \neq 0$:

$$\bar{u} = \overline{\sum_{\nu_1} g^\sigma[\nu_1, -\nu_1] \sum_{\nu_1} g^{-\sigma}[\nu_2, -\nu_2]}$$
$$= \sum_{\nu_1}\sum_{\nu_2} \overline{\bar{v}^\sigma_{\nu_1}\bar{v}^\sigma_{-\nu_1}\bar{v}^{-\sigma}_{\nu_2}\bar{v}^{-\sigma}_{-\nu_2}} \left(\frac{1}{2\pi}\right)^4 I^\sigma[\nu_1, -\nu_1] I^{-\sigma}[\nu_2, -\nu_2]$$
$$= \frac{(U\beta)^2}{8\pi^3}\sum_{\nu=1}^{\infty} I^\sigma[\nu, -\nu] I^{-\sigma}[\nu, -\nu]. \tag{4.7}$$

After simplification we have

$$I^\sigma[\nu, -\nu] = \frac{\delta}{\nu}\sum_{k=0}^{\nu-1}\frac{1}{(A^\sigma+1+k)(B^\sigma+\nu-k)}. \tag{4.8}$$

Some special cases are:

$$I^\sigma[1, -1] = \delta/(A^\sigma+1)(B^\sigma+1) \tag{4.9}$$

$$I^\sigma[2, -2] = (\delta/2)(1/(1+A^\sigma)(2+B^\sigma) + 1/(2+A^\sigma)(1+B^\sigma)). \tag{4.10}$$

At low temperature, expression (4.9) is consistent with the first harmonic approximation developed by Amit and Keiter [4]. It is worth noting that $I^\sigma[\nu, -\nu]$ must be permutation-invariant with respect to A^σ and B^σ. In fact we have

$$I^\sigma[\nu, -\nu] = \frac{\delta}{\nu(\delta+\nu)}\sum_{k=0}^{\nu-1}\left(\frac{1}{1+A^\sigma+k} + \frac{1}{1+B^\sigma+k}\right). \tag{4.11}$$

Our result (4.7) is useful and practicable in calculating the contribution from all the independent harmonics at low temperature.

Now let us further study how to consider the mixed mode effects. This is an important problem in FIA and has not yet been solved. But in this theoretical formalism, the mixed mode contributions appear in a natural way. All third diagrams are of mixed mode coherent effects. These diagrams can be calculated explicitly in our formalism.

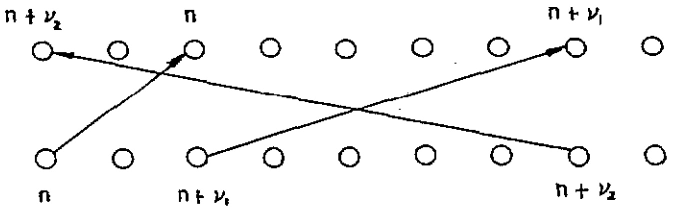

Figure 4. The lowest-order diagram with mixed modes.

In figure 4, a typical third-order diagram is shown with $\nu_2 \geqslant \nu_1 + 1$. The contribution of a general term with fixed ν_1, ν_2 is the following:

$$g^{\sigma}[\nu_1, \nu_2, -\nu_1 - \nu_2] = \tilde{v}^{\sigma}_{\nu_1}\tilde{v}^{\sigma}_{-\nu_2}\tilde{v}^{\sigma}_{\nu_2-\nu_1} \sum_{n=-\infty}^{\infty} \tilde{G}^{\sigma}_0(n)\tilde{G}^{\sigma}_0(n+\nu_1)\tilde{G}^{\sigma}_0(n+\nu_2)$$

$$= (\tilde{v}^{\sigma}_{\nu_1}\tilde{v}^{\sigma}_{-\nu_2}\tilde{v}^{\sigma}_{\nu_2-\nu_1}/(2\pi \mathrm{i})^3) I^{\sigma}[\nu_1, -\nu_2, \nu_2 - \nu_1] \tag{4.12}$$

where

$$I^{\sigma}[\nu_1, -\nu_2, \nu_2 - \nu_1] = \sum_{j=1}^{4} I^{\sigma}_{3j}$$

with

$$I^{\sigma}_{31} = \sum_{n=0}^{\infty} \frac{1}{(n+1+A^{\sigma})(n+1+\nu_1+A^{\sigma})(n+1+\nu_2+A^{\sigma})}$$

$$= \frac{1}{\nu_1\nu_2}\sum_{k=0}^{\nu_2-1}\frac{1}{A^{\sigma}+1+k} - \frac{1}{\nu_1(\nu_2-\nu_1)}\sum_{k=\nu_1}^{\nu_2-1}\frac{1}{A^{\sigma}+1+k} \tag{4.13}$$

$$I^{\sigma}_{32} = \sum_{n=-\nu_1}^{-1} \frac{1}{(n-B^{\sigma})(n+1+\nu_1+A^{\sigma})(n+1+\nu_2+A^{\sigma})}$$

$$= \frac{1}{\nu_2-\nu_1}\left[\left(\frac{1}{\delta+\nu_1} - \frac{1}{\delta+\nu_2}\right)\sum_{n=\nu_1}^{-1}\frac{1}{n-B^{\sigma}} - \frac{1}{\delta+\nu_1}\right.$$

$$\left.\times \sum_{n=-\nu_1}^{-1}\frac{1}{n+1+\nu_1+A^{\sigma}} + \frac{1}{\delta+\nu_2}\sum_{n=-\nu_1}^{-1}\frac{1}{n+1+\nu_2+A^{\sigma}}\right] \tag{4.14}$$

$$I^{\sigma}_{33} = \sum_{n=-\nu_2}^{-\nu_1-1} \frac{1}{(n-B^{\sigma})(n+\nu_1-B^{\sigma})(n+1+\nu_2+A^{\sigma})}.$$

$$= \frac{1}{\nu_1(\delta+\nu_2)}\sum_{n=-\nu_2}^{-\nu_1-1}\left(\frac{1}{n-B^{\sigma}} - \frac{1}{n+1+\nu_2+A^{\sigma}}\right)$$

$$-\frac{1}{\nu_1(\delta+\nu_2-\nu_1)}\sum_{n=-\nu_2}^{-\nu_1-1}\left(\frac{1}{n-B^\sigma+\nu_1}-\frac{1}{n+1+\nu_2+A^\sigma}\right) \tag{4.15}$$

and

$$I_{34}=\sum_{n=-\infty}^{-\nu_2-1}\frac{1}{(n-B^\sigma)(n+\nu_1-B^\sigma)(n+\nu_2-B^\sigma)}$$

$$=\frac{1}{\nu_1(\nu_2-\nu_1)}\sum_{k=\nu_2-\nu_1}^{\nu_2-1}\frac{1}{B^\sigma+1+k}-\frac{1}{\nu_2(\nu_2-\nu_1)}\sum_{k=0}^{\nu_2-1}\frac{1}{B^\sigma+1-k}. \tag{4.16}$$

one can express all these sums by a Ψ function or digamma functions as shown in mathematical references, such as Abramowitz and Stegun [10].

5. Some exact relations and expressions for the Anderson system

As applications of the functional-integral approach including mixed mode effects and free of divergence, in this section we try to prove some exact symmetry relations and expressions for the Anderson system by means of diagram analysis in FIA:

$$\chi(T,x_0,y_0)=\chi(T,1-x_0,y_0) \tag{5.1}$$

$$\bar{n}_l(T,1-x_0,y_0)=2-\bar{n}_l(T,x_0,y_0) \tag{5.2}$$

$$M(T,x_0,y_0,-\mathcal{H})=-M(T,x_0,y_0,\mathcal{H}) \tag{5.3}$$

where

$$x_0=-\varepsilon_l/U \qquad \delta=\Gamma/KT \qquad Y_0=U/\pi\Gamma. \tag{5.4}$$

The symmetry relations (5.1), (5.2) and (5.3) have been pointed out and proved in first harmonic approximation in FIA [2]. Recently they have also been proved in infinite harmonic approximation [1]. In this section we shall prove these relations to be exact.

Theorem. For the Anderson system, the functional-integral approach can prove that the symmetry relations (5.1), (5.2) and (5.3) are exact in any order.

Proof. According to the general diagram rules the partition function can be exactly expressed by [1]:

$$\Xi=f\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp(-\pi|z_0|^2)\,\mathrm{d}x_0\,\mathrm{d}y_0\left(\sum_k\bar{u}_k\prod_\sigma[\Gamma(1+A^\sigma)\Gamma(1+B^\sigma)]^{-1}\right). \tag{5.5}$$

In a magnetic field, we have

$$\varepsilon_{k\sigma}=\varepsilon_k-g_0\mu_B\sigma\mathcal{H} \qquad \varepsilon_{l\sigma}=\varepsilon_l-g\mu_B\sigma\mathcal{H} \tag{5.6}$$

where g and g_0 are Landé factors. Then

$$\bar{\varepsilon}_{l\uparrow}+\bar{\varepsilon}_{l\downarrow}-U/2=2\varepsilon_l+U/2 \tag{5.7}$$

are field-independent. The free energy is $F=-KT\ln\Xi$.

The magnetization M and susceptibility χ contributed from local states are

$$M = -\partial F/\partial \mathcal{H} = KT\,\Xi'/\Xi$$
$$\chi = (\partial M/\partial \mathcal{H})_{\mathcal{H}\to 0} = KT[\Xi''/\Xi - (\Xi'/\Xi)^2]. \tag{5.8}$$

According to the diagram rules, the partition function Ξ can be written as

$$\Xi = \sum_k \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}x_0\,\mathrm{d}y_0 \exp[-\pi(x_0^2 + y_0^2)] \prod_\sigma \Psi_k(A^\sigma, B^\sigma). \tag{5.9}$$

Because $\Psi_k(A^\sigma, B^\sigma)$ consist of the contributions of self-dual diagrams or dual diagrams, they both possess the following property:

$$\Psi_k(A^\sigma, B^\sigma) = \Psi_k(B^\sigma, A^\sigma). \tag{5.10}$$

Introducing

$$\xi = (\delta - 1)/2 \qquad b_\sigma = (\beta/2\pi)\bar{\varepsilon}_{l\sigma} \qquad a = \tfrac{1}{2}\sqrt{(U\beta/\pi)} \tag{5.11}$$

then

$$A^\sigma = \xi + \mathrm{i}b_\sigma - ay_0 + \mathrm{i}a\sigma x_0$$
$$B^\sigma = \xi - \mathrm{i}b_\sigma + ay_0 - \mathrm{i}a\sigma x_0. \tag{5.12}$$

So

$$\begin{aligned}\Xi[\xi, \{b_\sigma\}, a] &= \Big\langle \sum_k \prod_\sigma \Psi_k[A^\sigma, B^\sigma] \Big\rangle \\ &= \Big\langle \sum_k \prod_\sigma \Psi_k[\xi + \mathrm{i}b_\sigma + ay - \mathrm{i}\sigma ax; \xi - \mathrm{i}b_\sigma - ay + \mathrm{i}\sigma ax] \Big\rangle \\ &= \Big\langle \sum_k \prod_\sigma \Psi_k[\xi - \mathrm{i}b_\sigma - ay - \mathrm{i}\sigma ax; \xi + \mathrm{i}b_\sigma + ay - \mathrm{i}\sigma ax] \Big\rangle \\ &= \Xi[\xi, \{-b_\sigma\}, a]. \end{aligned} \tag{5.13}$$

The second step comes from the fact that Ξ is invariant under the inverse transformation of the dummy variables x_0 and y_0. The third step is due to the property of Ψ_k expressed by (5.10).

Then we have

$$\Xi[\xi, b_\uparrow, b_\downarrow, a] = \Xi[\xi, -b_\uparrow, -b_\downarrow, a]. \tag{5.14}$$

When $\mathcal{H} \to 0$, we have

$$b_\sigma = (\beta/2\pi)(\varepsilon_l + U/2) = b_l \qquad x_0 = -\varepsilon_l/U$$

so that

$$\Xi[\delta, x_0, y_0] = \Xi[\delta, 1 - x_0, y_0] \tag{5.15}$$

and therefore

$$\partial\Xi/\partial\mathcal{H} = -g\mu_\mathrm{B} \sum_\sigma \sigma\,\partial\Xi/\partial b_l. \tag{5.16}$$

Owing to the property (5.14),

$$\frac{\partial \Xi}{\partial \mathscr{H}} = g\mu_B \left(\frac{\partial}{\partial \omega_1} \Xi[\xi, \omega_1, -b_\downarrow, a] \bigg|_{\omega_1 = -b_\uparrow} - \frac{\partial}{\partial \omega_2} \Xi[\xi, -b_\uparrow, \omega_2, a] \bigg|_{\omega_2 = -b_\downarrow} \right).$$

Therefore

$$M[\xi, x_0, \mathscr{H}, y_0] = -M[\xi, 1 - x_0, -\mathscr{H}, y_0]. \tag{5.17}$$

When $\mathscr{H} \to 0$,

$$M[\xi, x_0, y_0] = -M[\xi, 1 - x_0, y_0] \tag{5.18}$$

where we have used the following properties: the odd-order derivatives of an even function are odd; the even-order derivatives of an even function are even. So

$$\lim_{\mathscr{H}\to 0} \frac{\partial^2}{\partial \mathscr{H}^2} \Xi[\xi, b_\uparrow, b_\downarrow, a] = (g\mu_B)^2 \sum_\sigma \frac{\partial^2}{\partial b_\sigma^2} \Xi[\xi, b_\sigma, b_{-\sigma}, a] \bigg|_{b_\sigma = b_{-\sigma} = b_l}$$

$$= (g\mu_B)^2 \sum_\sigma \frac{\partial^2}{\partial b_\sigma^2} \Xi[\xi, b_\sigma, b_{-\sigma}, a] \bigg|_{b_\sigma = b_{-\sigma} = -b_l}.$$

Therefore

$$\chi[\delta, 1 - x_0, y_0] = \chi[\delta, x_0, y_0]. \tag{5.19}$$

Now let us prove the exact relation (5.2). Denoting

$$\Xi = f\tilde{\Xi} \tag{5.20}$$

where

$$f = \Xi_{\text{band}} (2\pi)^2 \exp\left[-\frac{\beta}{2} \left(\sum_\sigma \varepsilon_{l\sigma} + \frac{U}{2} \right) \right] \tag{5.21}$$

it is obvious that

$$\bar{n}_k = -KT \frac{\delta}{\delta \varepsilon_k} \ln \Xi \tag{5.22}$$

$$\bar{n}_{l\sigma} = -KT \left(\frac{f'}{f} + \frac{\tilde{\Xi}'}{\tilde{\Xi}} \right) = -KT \frac{\delta}{\delta \varepsilon_l} \ln \Xi \tag{5.23}$$

and so

$$\bar{n}_{l\sigma}(\delta, x_0, y_0) = \tfrac{1}{2} - \frac{1}{2\pi} \tilde{\Xi}^{-1} \frac{d\tilde{\Xi}}{d\omega} [\xi, \omega, b_{-\sigma}, a] \bigg|_{\omega = b_\sigma}. \tag{5.24}$$

According to (5.14),

$$\frac{d}{d\omega} \tilde{\Xi}[\xi, \omega, b_{-\sigma}, a] \bigg|_{\omega = -b_l, b_{-\sigma} = -b_l} = -\frac{d}{d\omega} \tilde{\Xi}[\xi, \omega, b_{-\sigma}, a] \big|_{\omega = b_l, b_{-\sigma} = b_l}. \tag{5.25}$$

Then we have the exact relation

$$\bar{n}_{l\sigma}[\delta, 1 - x_0, y_0] = 1 - \bar{n}_{l\sigma}[\delta, x_0, y_0] \tag{5.26}$$

because

$$\bar{n}_l = \sum_\sigma \bar{n}_{l\sigma}$$
$$\bar{n}_l[\delta, 1 - x_0, y_0] = 2 - \bar{n}_l[\delta, x_0, y_0]. \tag{5.27}$$

For the symmetric case, the occupation number must be 1 exactly:

$$\bar{n}_l(\delta, x_0 = \tfrac{1}{2}, y_0] = 1. \tag{5.28}$$

According to the diagram analysis, one can also prove some exact expressions, which is useful in practical calculations.

Theorem. For the FIA, the susceptibility contributed by local states χ can be expressed exactly by

$$\chi = [4\pi(g\mu_B)^2/U](\bar{x}_0^2 - 1/2\pi) \tag{5.29}$$

where the average is defined by

$$\bar{A} = \frac{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp[-\pi(x_0^2 + y_0^2)]A(x_0, y_0)\Xi[x_0, y_0]\,\mathrm{d}x_0\,\mathrm{d}y_0}{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp[-\pi(x_0^2 + y_0^2)]\Xi[x_0, y_0]\,\mathrm{d}x_0\,\mathrm{d}y_0}. \tag{5.30}$$

The expression (5.29) has been derived in [4], with a factor missing.

Theorem. For the Anderson system one has exactly that

$$M[T, x_0, y_0, -\mathcal{H}] = -M[T, x_0, y_0, \mathcal{H}]. \tag{5.31}$$

Proof. Define

$$\Omega(\xi, b_{l\sigma}, b_{l-\sigma}, a, \mathcal{H}) \equiv \left\langle x_0 \sum_k \prod_\sigma \Psi_k[\xi + \mathrm{i}b_{l\sigma} - ay_0 + \mathrm{i}\sigma a x_0; \xi - \mathrm{i}b_{l\sigma} + ay_0 - \mathrm{i}a\sigma x_0]\right\rangle \tag{5.32}$$

then

$$\Omega(\xi, b_{l\sigma}, b_{l-\sigma}, a, -\mathcal{H}) = \left\langle x_0 \sum_k \prod_\sigma \Psi_k[\xi + \mathrm{i}\, b_{l-\sigma} - ay_0 + \mathrm{i}\,\sigma a x_0; \xi - \mathrm{i}\, b_{l\sigma} + ay_0 + \mathrm{i}\, a\sigma x_0]\right\rangle. \tag{5.33}$$

Using equation (5.10) and the transformations $x_0 \to -x$, $\sigma \to -\sigma$, we have

$$\Omega(\xi, b_{l\sigma}, b_{l-\sigma}, a, -\mathcal{H}) = -\Omega(\xi, b_{l\sigma}, b_{l-\sigma}, a, \mathcal{H}) \tag{5.34}$$

and since

$$M = -KT\frac{\partial}{\partial\mathcal{H}}\ln\Xi$$

we obtain

$$M(T, x_0, y_0, -\mathcal{H}) = -M(T, x_0, y_0, \mathcal{H}). \tag{5.35}$$

The theorem is proved.

Please notice that:

(i) One of the benefits of our diagram analysis is that we can preserve all the exact symmetry relations in every step(stage).

(ii) In practical calculations, these relations and expressions are useful. For example, knowing the partition function, including the higher-order diagram contribution to calculate the susceptibility, one usually needs the second derivatives of Ξ with a lot of terms. But if we start from (5.29), then we only need one term.

6. On the Anderson system with attractive Coulomb interaction

The Anderson system with attractive Coulomb interaction is very interesting. Sometimes it has been considered to be related with superconductivity. In this section we try to generalize the previous results to the negative U case:

$$U = -U_0 < 0. \tag{6.1}$$

We have

$$\begin{aligned} a_0 &= \tfrac{1}{2}\surd(U_0\beta/\pi) \qquad & a &= \mathrm{i}\, a_0 \\ b_{l\sigma} &= (\beta/2\pi)(\varepsilon_{l\sigma} - U_0/2) \qquad & \xi &= (\delta - 1)/2. \end{aligned} \tag{6.2}$$

Following a similar discussion to that in section 5, we can also obtain the same relations of the partition function Ξ, susceptibility χ, occupation number $\bar{n}_l$ and magnetization M for the negative U case:

$$\begin{aligned} &\Xi[-U_0, \delta, y_0, 1 - x_0] = \Xi[-U_0, \delta, y_0, x_0] \\ &\chi[-U_0, \delta, y_0, 1 - x_0] = \chi[-U_0, \delta, y_0, x_0] \\ &\bar{n}_l[-U_0, \delta, y_0, 1 - x_0] = 2 - \bar{n}_l[-U_0, \delta, y_0, x_0] \\ &M[-U_0, \delta, y_0, 1 - x_0, \mathcal{H}] = -M[-U_0, \delta, y_0, x_0, -\mathcal{H}]. \end{aligned} \tag{6.3}$$

The special cases are:

$$\lim_{\mathcal{H}\to 0} M[-U_0, \delta, y_0, x_0, \mathcal{H}] = 0 \tag{6.4}$$

$$\bar{n}_l[-U_0, \delta, y_0, x_0 = \tfrac{1}{2}, \mathcal{H}] = 1. \tag{6.5}$$

It is very interesting to note that the exact occupation number expressions for the Anderson systems with repulsive and attractive Coulomb interactions are different.

An exact expression for the occupation number for the Anderson system with $U = -U_0$ is:

$$\bar{n}_{l\sigma} = \tfrac{1}{2} + [2\pi/\surd(U_0\beta\pi)]\bar{y}_0. \tag{6.6}$$

We prove this as follows. For $U = -U_0 < 0$, letting

$$y = y_0 - b_{l\sigma}/a_0 \tag{6.7}$$

one obtains

$$\begin{aligned} \Xi[-U_0, \xi, b_{l\sigma}, b_{l-\sigma}, a_0] = \sum_k \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp\left\{-\pi\left[\left(y + \frac{b_{l\sigma}}{a_0}\right)^2 + x_0^2\right]\right\} \\ \times \mathrm{d}x_0\, \mathrm{d}y \prod_\sigma \Psi_k[-U_0, \xi - \mathrm{i}a_0 y - \sigma a_0 x_0; \xi + \mathrm{i}a_0 y + \sigma a_0 x_0]. \end{aligned} \tag{6.8}$$

Notice that the transformation (6.7) is only applicable to the zero-field case, or it will be σ-dependent. So we discuss the occuption number in zero field:

$$\bar{n}_{l\sigma} = -KT(f'/f + \bar{\Xi}'/\bar{\Xi}) \tag{6.9}$$

$$\bar{\Xi}' = -2\pi\sqrt{\left(\frac{\beta}{U_0\pi}\right)} \sum_k \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} y_0 \exp[-\pi(x_0^2 + y_0^2)] \prod_\sigma \Psi_k(A^\sigma, B^\sigma). \tag{6.10}$$

Then we obtain the exact expression (6.6). This expression is also useful in proving relation (6.3) and in practical calculations.

7. Discussion and concluding remarks

Two of the main problems in the functional-integral approach are how to overcome the divergence difficulty and how to calculate the contributions from mixed modes. In this paper we discussed the causes of mathematical breakdown of RPA'. One is due to the limitation of the expansion formula used; the other is due to the improper approximation of the determinants. Unlike the usual theory of FIA, we analyse and prove the validity condition of a matrix formula and point out that its benefits are its independent expansion form and the fact that there is no problem of limitation of convergence radius. Starting from this formula and exact rules for a determinant, we establish a diagram analysis of FIA, with the following characteristics:

(i) There is no divergence and no problem of limitation of convergence radius. This is different from another approach [6].

(ii) The reality of partition functions in every stage is guaranteed, even in the complex representation, and all the benefits of the complex representation are preserved.

(iii) All the functional-integral series are transformed into finite-dimensional (2D) integrals.

(iv) The contributions of mixed mode effects are included in a natural way. It is the first time that a concrete calculating method has been given.

(v) According to the diagram analysis of FIA, we prove some exact relations (5.1), (5.2), (5.3) and (5.28) for $U > 0$ and (6.3), (6.4) and (6.5) for $U < 0$.

(vi) We also give and prove an exact expression for the occupation number (6.6) for negative U, which corresponds to the exact susceptibility expression (5.29) for positive U. They are useful in practical calculations and in the proof of some exact symmetry relations.

Other related topics will be discussed later [9].

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