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VARIATIONAL APPROACH TO CORRELATION FUNCTIONS AND TO THE PERIODIC ANDERSON MODEL IN INFINITE DIMENSIONS

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INTRODUCTION

Theoretical investigations of strongly correlated electronic systems in the thermodynamic limit, as described for example by the Hubbard model¹ or the periodic Anderson model,² are conventionally plagued by severe computational problems. These increase drastically with dimension and therefore one often resorts to investigations of one-dimensional systems, hoping that they are able to provide essential insight into higher-dimensional systems. Recently Metzner and Vollhardt³ showed that, for quantum mechanical models of itinerant electrons such as the Hubbard model, the limit of infinite dimensions ($d = \infty$) provides for another useful approach. Above all, in the case of $d = \infty$ drastic calculational simplifications arise, while at the same time correlations remain non-trivial provided a proper scaling of the model with the dimension d is taken into account. –

In this paper we extend the earlier investigations in $d = \infty$ which concentrated on the ground state energy of the Hubbard model.³ Firstly, correlation functions for Hubbard-type models are evaluated analytically in terms of the Gutzwiller wave function (GWF) without approximation.⁴ This shows that non-trivial correlations may indeed exist even in $d = \infty$. Secondly, the periodic Anderson model is investigated in terms of a suitable generalization of the GWF in $d = \infty$. It is shown that the evaluations can be performed analytically, too, and that the results agree with those obtained earlier⁵ by employing (semi-)classical counting arguments in the spirit of the so-called “Gutzwiller approximation”.^{6,7} Hence these (semi-)classical methods are found to yield the correct results in $d = \infty$ for the variational wave functions under consideration.

THE VARIATIONAL APPROACH

Here we consider variational investigations of models, whose interaction is purely on-site, i.e. only takes place between electrons of opposite spin on the same lattice site

$$\hat{H} = U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow} \quad (1)$$

where $\hat{n}_{\mathbf{i}\sigma}$ is the number operators for a spin at site \mathbf{i} and

$$\hat{D} = \sum_{\mathbf{i}} \hat{D}_{\mathbf{i}} = \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow} \quad (2)$$

is the number operator for doubly occupied sites. To evaluate expectation values $\langle \hat{O} \rangle = \langle \Psi | \hat{O} | \Psi \rangle / \langle \Psi | \Psi \rangle$ of operators \hat{O} occurring in models containing (1), we employ generalizations of the GWF⁶, i.e.

$$| \Psi \rangle = g^{\hat{D}} | \Phi_0 \rangle \quad (3a)$$

$$= \prod_i [1 - (1 - g)\hat{D}_i] | \Phi_0 \rangle \quad (3b)$$

Here $0 \leq g \leq 1$ is a variational parameter such that the correlation operator $g^{\hat{D}}$ suppresses unfavourable spin configurations within a suitably chosen starting wave function $| \Phi_0 \rangle$. For $| \Phi_0 \rangle = | FS \rangle$, the Fermi sea, (3) reduces to the original GWF⁶

$$| \Psi_G \rangle = g^{\hat{D}} | FS \rangle \quad (4)$$

A general theoretical approach to the evaluation of expectation values $\langle \hat{O} \rangle$ in terms of $| \Psi_G \rangle$ has recently been formulated.⁸ It is based on an expansion of $\langle \hat{O} \rangle$ in powers of $(g^2 - 1)$, where the coefficients can be determined diagrammatically using standard field theoretical methods. Their evaluations is greatly simplified by use of special contractions, which only involve anticommuting numbers as in a Grassmann algebra. In this way exact, analytic evaluations are possible in $d = 1$ for arbitrary densities and interaction strengths. Diagrams in this formalism are made up of lines connecting sites i and j , which correspond to

$$P_{\sigma,ij}^0 = \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \rangle_0 \quad (5)$$

where $\langle \hat{O} \rangle_0 = \langle FS | \hat{O} | FS \rangle$, and of point vertices. –

In $d = \infty$ $P_{\sigma,ij}^0$ has the property³

$$P_{\sigma,ij}^0 \leq \mathcal{O}\left(\frac{1}{\sqrt{d}}\right) \quad i \neq j \quad (6)$$

which causes a collapse of diagrams in which vertices i and j are connected by three or more separate paths. This leads to tremendous simplifications in the diagrammatic calculation of expectation values and thereby allows for exact evaluations of the ground state energy of the Hubbard model in $d = \infty$ in terms of increasingly refined variational wave functions.³

CORRELATION FUNCTIONS

There are four independent correlation functions for Hubbard-type models

$$C_f^{XY} = \frac{1}{L} \sum_{\mathbf{h}} \langle \hat{X}_{\mathbf{h}} \hat{Y}_{\mathbf{h}+\mathbf{f}} \rangle - \langle \hat{X} \rangle \langle \hat{Y} \rangle \quad (7)$$

where $\langle \hat{X} \rangle = L^{-1} \sum_i \hat{X}_i$, with L as the number of lattice sites, and \hat{X}_i, \hat{Y}_i correspond to the spin $\hat{S}_i^z (= \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$, density $\hat{N}_i (= \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})$, hole $\hat{H}_i (= (1 - \hat{n}_{i\uparrow})(1 - \hat{n}_{i\downarrow}))$ or double occupancy $\hat{D}_i (= \hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$. These correlation functions were recently calculated by us in terms of the GWF for $d = 1$ in closed form.⁹

Exact evaluations are also possible in $d = \infty$. To be able to exploit the simplifications in the diagrammatic calculation of (7) arising from (6), we have to separate out those parts of the graphs in which vertices are connected by three or more separate paths. This procedure will now be exemplified in the case of the spin-spin correlation function C_j^{XY} . Noting that

the external vertices of diagrams contributing by C_j^{XY} are only connected to two lines each, we introduce a 4-point vertex function $\Gamma_{\sigma,\sigma'}(1,2,3,4)$, where $i \equiv f_i$ etc. , such that C_j^{SS} is given by

$$C_j^{SS} = \frac{1}{L} \sum_{\sigma} \sum_{\mathbf{f}} \left\{ -(P_{\sigma;\mathbf{f},\mathbf{f}+\mathbf{j}})^2 + P_{\sigma;\mathbf{f},\bar{1}} P_{\sigma;\mathbf{f},\bar{2}} \Gamma_{\sigma,\sigma}(\bar{1},\bar{2},\bar{3},\bar{4}) P_{\sigma;\bar{3},\mathbf{f}+\mathbf{j}} P_{\sigma;\bar{4},\mathbf{f}+\mathbf{j}} \right. \\ \left. - P_{\sigma;\mathbf{f},\bar{1}} P_{\sigma;\mathbf{f},\bar{2}} \Gamma_{\sigma,-\sigma}(\bar{1},\bar{2},\bar{3},\bar{4}) P_{-\sigma;\bar{3},\mathbf{f}+\mathbf{j}} P_{-\sigma;\bar{4},\mathbf{f}+\mathbf{j}} \right\} \\ + \delta_{j,0} \left[n - 2\bar{d} \frac{1-g^2}{g^2} \right] + \frac{1}{L} \sum_{\mathbf{f}} (n_{\mathbf{f},\uparrow} - n_{\mathbf{f}+\mathbf{j},\downarrow})^2 - \left[\frac{1}{L} \sum_{\mathbf{f}} (n_{\mathbf{f},\uparrow} - n_{\mathbf{f},\downarrow}) \right]^2 \quad (8)$$

where $n_{\sigma} = n_{\uparrow} + n_{\downarrow}$ is the particle density and $\bar{d} = \langle \hat{D} \rangle / L$ is the density of doubly occupied sites.⁹ Here a full line between two vertices \mathbf{f} , \mathbf{g} is taken as a dressed fermion line, which contains all self-energy insertions, and corresponds to a factor $P_{\sigma;\mathbf{f},\mathbf{g}}$.³ As usual indices with a bar (\bar{h} , $\bar{1} = \bar{f}_1$, etc.) are summed over. The (two-particle) irreducible 4-point vertex $\Gamma_{\sigma,\sigma'}^*(1,2,3,4)$ is implicitly obtained from $\Gamma_{\sigma,\sigma'}$ as

$$\Gamma_{\sigma,\sigma'}(1,2,3,4) = \Gamma_{\sigma,\sigma'}^*(1,2,3,4) - \Gamma_{\sigma,\sigma'}^*(1,2,\bar{3},\bar{4}) P_{\sigma';\bar{3},\bar{1}} P_{\sigma';\bar{4},\bar{2}} \Gamma_{\sigma',\sigma'}(\bar{1},\bar{2},3,4) \\ - \Gamma_{\sigma,-\sigma'}^*(1,2,\bar{3},\bar{4}) P_{-\sigma';\bar{3},\bar{1}} P_{-\sigma';\bar{4},\bar{2}} \Gamma_{-\sigma',\sigma'}(\bar{1},\bar{2},3,4) \quad (9)$$

Clearly, all vertices contained in Γ^* are now connected with each other by three or more separate paths and hence collapse in $d = \infty$, such that

$$\Gamma_{\sigma,\sigma'}^*(1,2,3,4) \equiv \delta_{1,2} \delta_{1,3} \delta_{1,4} \tilde{\Gamma}_{\sigma,\sigma'}^*(1) \quad (10)$$

which defines a local quantity $\tilde{\Gamma}_{\sigma,\sigma'}^*(\mathbf{j})$. This implies $\Gamma_{\sigma,\sigma'}(1,2,3,4) \equiv \delta_{1,2} \delta_{3,4} \tilde{\Gamma}_{\sigma,\sigma'}(1,3)$ for the vertex-function itself. The quantities $\tilde{\Gamma}_{\sigma,\sigma'}^*(\mathbf{j})$ are easily determined from the value of the correlation function at $\mathbf{j} = 0$.

The above formalism is valid for arbitrary starting wave functions $|\Phi_0\rangle$ in (3). In particular, for the GWF with $|\Phi_0\rangle = |FS\rangle$ and $n_{\uparrow} = n_{\downarrow} = n/2$ all calculations are greatly simplified due to translational invariance and spin-symmetry. For example $\tilde{\Gamma}_{\sigma,\sigma'}^*(\mathbf{f})$ reduce to mere constants ($\tilde{\Gamma}_{\sigma,\sigma}^* = \tilde{\Gamma}_{-\sigma,-\sigma}^* \equiv \Gamma_1$, $\tilde{\Gamma}_{\sigma,-\sigma}^* = \tilde{\Gamma}_{-\sigma,\sigma}^* \equiv \Gamma_2$), such that the equations for $\Gamma_{\sigma,\sigma'}$, (9), are easy to solve. The momentum-dependent spin-spin correlation function is then found as⁴

$$C^{SS}(\mathbf{k}, n, g) = \frac{C_0(\mathbf{k}, n)}{1 - V_S(g, n) C_0(\mathbf{k}, n)} \quad (11)$$

where $C_0(\mathbf{k}, n) = C^{SS}(\mathbf{k}, n, 1)$ is the result for the noninteracting case ($g = 1$) and

$$V_S = \frac{1}{n - 2\bar{d}} - \frac{1}{n - 2\bar{d}_0} \quad (12)$$

The mean double occupancy \bar{d} has been calculated earlier as³

$$\bar{d}(g, n_{\uparrow}, n_{\downarrow}) = \frac{1 + n(g^2 - 1) - \sqrt{1 - (1 - g^2)[n(2 - n) + g^2(n^2 - 4\bar{d}_0)]}}{2(g^2 - 1)} \quad (13)$$

where $\bar{d}_0 = n_{\uparrow} n_{\downarrow}$ and $n = n_{\uparrow} + n_{\downarrow}$. It is interesting to note that in $d = \infty$ the correlation function C^{SS} does not reduce to some trivial result, as might have been expected. The RPA-like structure of (11) is due to the summation of dressed bubble-diagrams, which are the only

ones that survive in $d = \infty$. (This finding is expected to be true even for the exact solution of the Hubbard model in $d = \infty$). The quantity V_S corresponds to a renormalized coupling constant. — Other correlation functions, such as C^{NN} , C^{DN} , C^{DD} , are obtained by the same procedure and are found to have the same structure as that of C^{SS} .⁴ —

The Fourier transformation of (11) into position space ($C^{SS}(\mathbf{k}) \rightarrow C_{\mathbf{j}}^{SS}$) is a delicate problem in view of the integration involved and the two limits $L \rightarrow \infty, d \rightarrow \infty$, which do not commute. Nonetheless, $C_0(\mathbf{k}, n)$ can be calculated explicitly in $d = \infty$ ⁴ and the Fourier retransformation is achieved by noting that for almost all \mathbf{k} -values $C_0(\mathbf{k}, n)$ assumes the average value $\langle C_0(\mathbf{k}, n) \rangle_{\mathbf{k}} = n(1 - n/2)$, such that (11) can be expanded in the quantity $C_0(\mathbf{k}, n) - \langle C_0(\mathbf{k}, n) \rangle_{\mathbf{k}}$, which is small for almost all \mathbf{k} . In zeroth order one obtains $C_{\mathbf{j}=0}^{SS} = n - 2\bar{d}$, while the nearest-neighbor contribution to $\mathbf{j} = 0$ is obtained by the first order term as

$$C_{\mathbf{j}=n.n.}^{SS}(g, n) = \frac{C_{\mathbf{j}=n.n.}^{SS}(1, n)}{[1 - V_S(g, n)\langle C_0(\mathbf{k}, n) \rangle_{\mathbf{k}}]^2} \quad (14a)$$

$$= \left(\frac{n - 2\bar{d}}{n - 2d_0} \right)^2 C_{\mathbf{j}=n.n.}^{SS}(1, n) \quad (14b)$$

This shows that, at least for nearest-neighbors, the correlation function for the interacting case is proportional to that for the non-interacting case. This result had been derived earlier⁵ by (semi-)classical counting arguments in the spirit of the Gutzwiller approximation^{6,7}. Here we are able to show that for the GWF this result is exact in high dimensions ($d = \infty$). In fact, numerical investigations⁵ indicate that (14) is well obeyed even in $d = 2$. Hence we learn that results for high dimensions are able to give essential insight into the behavior of much lower-dimensional systems.

PERIODIC ANDERSON MODEL (PAM)

This model is generally considered appropriate for a description of the physics of heavy fermion systems.² It considers almost localized f -shell electrons on a periodic lattice (with lattice sites essentially singly occupied due to the strong intraatomic Coulomb repulsion), in a sea of conduction electrons (c) with a finite hybridization between c 's and f 's: In the absence of orbital degeneracy it has the form

$$\begin{aligned} \hat{H}_{PAM} = & \sum_{\mathbf{k}\sigma} \epsilon_c(\mathbf{k}) \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \epsilon_f(\mathbf{k}) \hat{f}_{\mathbf{k}\sigma}^\dagger \hat{f}_{\mathbf{k}\sigma} \\ & + U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}\uparrow}^f \hat{n}_{\mathbf{i}\downarrow}^f - \sum_{\mathbf{k}\sigma} [V_{\mathbf{k}} \hat{f}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + h.c.] \end{aligned} \quad (15)$$

The first two terms describe the band behavior of c - and f -electrons, the third is the Hubbard term (1) for the f 's (being the only interaction term in \hat{H}_{PAM}) and the last term produces the quantum mechanical mixing. For $U = 0$ (15) is easily diagonalized and yields for less than half filling ($n_\uparrow + n_\downarrow \leq 2$)^{10,11}

$$|\Psi\{a_\sigma^0(\mathbf{k})\}\rangle = \prod_{\sigma} \prod_{|\mathbf{k}| \leq k_F^c} [1 + a_\sigma^0(\mathbf{k}) \hat{f}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma}] |cFS\rangle \quad (16)$$

where $|cFS\rangle$ is the Fermi sea of c -electrons and

$$a_\sigma^0(V_{\mathbf{k}}, \epsilon_f(\mathbf{k})) \equiv a_\sigma^0(\mathbf{k}) = \frac{2V_{\mathbf{k}}}{\epsilon_f(\mathbf{k}) - \epsilon_c(\mathbf{k}) + [(\epsilon_f(\mathbf{k}) - \epsilon_c(\mathbf{k}))^2 + 4V_{\mathbf{k}}^2]^{1/2}} \quad (17)$$

For a variational investigation of the interacting problem, a wave function of the form given by (3) has been suggested^{10,11,12},

$$|\Psi_{PAM}\rangle = g^{\hat{D}^f} |\Psi\{a_\sigma(\mathbf{k})\}\rangle \quad (18)$$

where now $\hat{D} \equiv \hat{D}^f = \sum_i \hat{n}_{i\uparrow}^f \hat{n}_{i\downarrow}^f$ and $a_\sigma^0(\mathbf{k})$ has been replaced by some function $a_\sigma(\mathbf{k})$, which has to be determined variationally.

To evaluate expectation values in terms of $|\Psi_{PAM}\rangle$ it is essential to note that the Gutzwiller correlation operator acts only on the f -electrons. Therefore it is possible to express all expectation values in terms of the f -electron self-energy S_σ , which itself depends only on the properties of the f -electrons. In this situation one may simply take over the results obtained earlier within the ordinary GWF³ for the Hubbard model. In particular, construction of the proper self-energy S_σ^* via the Dyson equation leads to a collapse of diagrams in $d = \infty$, such that S_σ^* becomes site-diagonal. The remaining local quantity is obtained by summing the skeleton expansion, which can be performed exactly in $d = \infty$. The results for the Hubbard model, using the GWF, (4), and for the PAM in terms of $|\Psi_{PAM}\rangle$ are then very similar. For example, the relation between \bar{d}^f , the average double occupancy for f -electrons, and the variational parameter g is given by (13) with $\bar{d} \rightarrow \bar{d}^f$ and $n_\sigma \rightarrow n_\sigma^f$. The main differences are that the number of f -electrons, n_σ^f , is not conserved, i.e. depends on g and $a_\sigma(\mathbf{k})$, and that fermion lines $P_{\sigma,ij}^0$, (5), for the f 's have a more complicated structure. In spite of this the expectation value $\langle \hat{H}_{PAM} \rangle$ can be calculated exactly in $d = \infty$. Thereby we derive the results obtained earlier by (semi-)classical counting arguments à la Gutzwiller¹⁰⁻¹³ (for the most complete treatment see ref. 14), which are therefore seen to be strictly correct in high dimensions. In $d = \infty$ the correlation operator in (18) leads to a simple renormalization of one-particle quantities, e.g.

$$\begin{aligned} V_{\mathbf{k}} &\rightarrow \tilde{V}_{\mathbf{k}} = \sqrt{q_\sigma} V_{\mathbf{k}} \\ \epsilon_f(\mathbf{k}) &\rightarrow \tilde{\epsilon}_f(\mathbf{k}) = q_\sigma \epsilon_f(\mathbf{k}) + shift \\ a_\sigma(\mathbf{k}) &\rightarrow \tilde{a}_\sigma(\mathbf{k}) = \sqrt{q_\sigma} a_\sigma^0(\tilde{V}_{\mathbf{k}}, \tilde{\epsilon}_f(\mathbf{k})) \end{aligned} \quad (19)$$

where q_σ is the correlation-induced reduction in the kinetic energy (the “discontinuity” of the momentum distribution in the case of the Hubbard model), which for $U = \infty$ is given by

$$q_\sigma = \frac{1 - (n_\uparrow^f + n_\downarrow^f)}{1 - n_\sigma^f} \quad (20)$$

This shows that one may indeed construct an effective Hamiltonian defined in terms of the renormalized quantities $\tilde{V}_{\mathbf{k}}, \tilde{\epsilon}_f(\mathbf{k})$, as anticipated by Rice and Ueda¹⁰. The results derived above for $d = \infty$ also agree with those obtained by a slave boson approach to the PAM via a path integral method.¹⁵

CONCLUSION

Using variational wave functions explicit analytic results have been obtained for correlation functions and the periodic Anderson model in the limit of infinite dimensions. Correlations are found to remain non-trivial. Semi-classical counting methods, frequently used for an approximate evaluation of expectation values in lower dimensional systems, were shown to become exact in $d = \infty$.

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REFERENCES

1. M. C. Gutzwiller, Phys. Rev. Lett. **10** (1963); J. Hubbard, Proc. R. Soc. London **A276** 238 (1963); J. Kanamori, Prog. Theor. Phys. **30** 275 (1973)
2. See, for example, P. A. Lee, T. M. Rice, J. W. Serene, L. J. Sham and J. W. Wilkins, Comments Cond. Matt. Phys. **XII**, 99 (1986)
3. W. Metzner and D. Vollhardt, Phys. Rev. Lett. , in press (January 16, 1989); see also the accompanying article by these authors in this volume of the NATO proceedings
4. For details, see F. Gebhard, P. van Dongen and D. Vollhardt, preprint RWTH/ITP-C 14/88 , to be published
5. F. C. Zhang, C. Gros, T. M. Rice and H. Shiba; Supercond. Science and Techn. **1** 36 (1988)
6. M. C. Gutzwiller, Phys. Rev. **A137** 1276 (1965)
7. D. Vollhardt, Rev. Mod. Phys. **56** 99 (1984)
8. W. Metzner and D. Vollhardt, Phys. Rev. Lett. **59** 121 (1987); Phys. Rev. **B37** 7382 (1988)
9. F. Gebhard and D. Vollhardt, Phys. Rev. Lett. **59** 1472 (1987); Phys. Rev. **B38** 6911 (1988)
10. T. M. Rice, K. Ueda, Phys. Rev. Lett. **55** 995 (1985); Phys. Rev. **B34** 6420 (1986)
11. B. H. Brandow, Phys. Rev. **B33** 215 (1986)
12. C. M. Varma, W. Weber and L. J. Randall, Phys. Rev. **B33** 1015
13. P. Fazekas and B. H. Brandow, Physica Scripta **36** 809 (1987)
14. V. Z. Vulović and E. Abrahams, Phys. Rev. **B36** 2614 (1987)
15. G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. **57** 1362 (1986)