Variational evaluation of correlation functions for lattice electrons in high dimensions

P.G.J. van Dongen, F. Gebhard, and D. Vollhardt
Institut für Theoretische Physik C, Technische Hochschule Aachen,
Federal Republic of Germany

We present a general formalism for the diagrammatic calculation of correlation functions for Hubbard-type models in terms of projected wave functions. It is shown that in the limit of high spatial dimensions d only diagrams with bubble-structure remain. This causes correlation functions to have an overall RPA-type form in $d \to \infty$. Exact evaluations are performed for the Gutzwiller wave function. Nearest neighbor correlations are shown to be proportional to their value in the non-interacting case, i.e. are renormalized. However, their absolute value is only of order $1/d$. Hence this wave function does not describe spin correlations adequately in high dimensions. The asymptotic behavior of the spin-correlation function is extracted and is found to have a scaling form similar to $d=1$. Assuming this form to hold in all dimensions we show that the Brinkman-Rice transition only occurs in $d=\infty$. Finite orders of perturbation theory in $1/d$ around this singular point are not sufficient to remove the transition.

I. Introduction

Correlation functions (CFs) contain particularly rich information about the nature of a physical system. Therefore it is not surprising that by the same token their analytic evaluation is in general a difficult – if not insurmountable – theoretical problem. For example, even for the antiferromagnetic Heisenberg model in dimension $d=1$ the spin-spin correlation function is only known in limiting cases [1–3]. In the case of the Hubbard model [4], which reduces to the former model in the limit $U \to \infty$ and half-filling ($n=1$), the situation is therefore even worse. In spite of the exact solution for the ground state energy [5], exact, analytic results for CFs at intermediate U and/or $n<1$ are not available. In this situation variational wave functions (VWFs) have been a very useful tool for studying these models [6]. Even in this approximate approach analytic results are difficult to obtain. – Recently, Metzner and Vollhardt [7] introduced the limit of high dimensions ($d \to \infty$) of the Hubbard-model. They showed that in this limit the model, when scaled properly, remains non-trivial, while at the same time diagrammatic treatments become substantially simpler, allowing even for analytic calculations. In the present paper we use this approach to evaluate correlation functions (CFs) of the Hubbard-model in terms of a general class of variational wave functions. – The general structure of the CFs and their diagrammatic representation is discussed in Sect. II and III. Explicit evaluations in $d=\infty$ are presented in Sect. IV, in particular for the Gutzwiller wave function. Restricting the discussion to the latter wave function, nearest neighbor correlations are evaluated in Sect. V. The behavior beyond nearest neighbors and the asymptotic behavior, is determined in Sect. VI. Employing scaling arguments these results are used in Sect. VII to show that a Brinkman-Rice transition will not occur at any finite dimension but only in $d=\infty$. A conclusion is presented in Sect. VIII.

II. Correlation functions for the Hubbard model

In the Hubbard model [4], $\hat{H}=\hat{H}_{\text{kin}}+\hat{H}_I$, the kinetic energy is given by

$$\hat{H}_{\text{kin}}=\sum_{\langle \mathbf{ij}\rangle}\sum_{\sigma} t_{\mathbf{ij}}\hat{c}^+_{\mathbf{i}\sigma}\hat{c}_{\mathbf{j}\sigma}=\sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}\hat{n}_{\mathbf{k}\sigma} \qquad (1)$$

in position and momentum space, respectively. Here $\hat{n}_{\mathbf{k}\sigma}=\hat{a}^+_{\mathbf{k}\sigma}\hat{a}_{\mathbf{k}\sigma}$ is the momentum distribution operator (in the following operators always carry a hat ^) and

$$\varepsilon_{\mathbf{k}}=-2t\sum_{i=1}^{d}\cos k_i, \qquad t=\bar{t}/\sqrt{2d} \tag{2}$$

is the energy dispersion for nearest neighbor hopping on a d-dimensional hypercubic lattice with unit spacing. The scaling of the hopping constant, $t\to t=\bar{t}/\sqrt{2d}$ with $\bar{t}$ fixed, guarantees that the average kinetic energy remains finite even for $d\to\infty$ [7]. The interaction has the form

$$\hat{H}_I=U\sum_{\mathbf{i}}\hat{n}_{\mathbf{i}\uparrow}\hat{n}_{\mathbf{i}\downarrow}=U\hat{D} \tag{3}$$

where $\hat{D}=\sum_{\mathbf{i}}\hat{D}_{\mathbf{i}}$ and $\hat{D}_{\mathbf{i}}=\hat{n}_{\mathbf{i}\uparrow}\hat{n}_{\mathbf{i}\downarrow}$ is the operator for double occupancy of a site $\mathbf{i}$ by two electrons with opposite spins.

A typical VWF for the study of $\hat{H}$ is

$$|\Psi\rangle=g^{\hat{D}}|\Phi_0\rangle=\prod_{\mathbf{i}}[1-(1-g)\hat{D}_{\mathbf{i}}]|\Phi_0\rangle \tag{4}$$

with $|\Phi_0\rangle$ as an arbitrary one-particle wave function, which need not be translationally invariant, and $0\leqq g\leqq 1$ is a variational parameter. This is a generalization of the Gutzwiller wave function [4, 8]

$$|\Psi_G\rangle=g^{\hat{D}}|\mathrm{FS}\rangle \tag{5}$$

where $|\Phi_0\rangle=|\mathrm{FS}\rangle$ is the paramagnetic Fermi sea. A new analytic approach for the evaluation of expectation values $\langle\hat{O}\rangle=\langle\Psi|\hat{O}|\Psi\rangle/\langle\Psi|\Psi\rangle$ for an operator $\hat{O}$ in terms of $|\Psi_G\rangle$ has recently been introduced by Metzner and Vollhardt [9]. In particular, CFs for Hubbard-type models

$$C^{XY}_{\mathbf{j}}=\frac{1}{L}\sum_{\mathbf{i}}\langle\hat{X}_{\mathbf{i}}\hat{Y}_{\mathbf{i}+\mathbf{j}}\rangle-\langle\hat{X}\rangle\langle\hat{Y}\rangle \tag{6}$$

where $\hat{X}=L^{-1}\sum_{\mathbf{i}}\hat{X}_{\mathbf{i}}$ and L is the number of lattice sites, have been evaluated exactly in $d=1$ for arbitrary densities and correlation strengths [10]. Here $\hat{X}_{\mathbf{i}}$, $\hat{Y}_{\mathbf{i}}$ correspond to the respective operators for the spin $\hat{S}^z_{\mathbf{i}}(=\hat{n}_{\mathbf{i}\uparrow}-\hat{n}_{\mathbf{i}\downarrow})$, density $\hat{N}_{\mathbf{i}}(=\hat{n}_{\mathbf{i}\uparrow}+\hat{n}_{\mathbf{i}\downarrow})$, a hole $\hat{H}_{\mathbf{i}}(=(1-\hat{n}_{\mathbf{i}\uparrow})(1-\hat{n}_{\mathbf{i}\downarrow}))$ or a doubly occupied site $\hat{D}_{\mathbf{i}}$. Of the possible combinations only four CFs are independent, e.g. C^{SS}, C^{NN}, C^{ND}, C^{DD}.

The approach presented in [9, 10] also holds in the case of generalized projected wave functions $|\Psi\rangle$, (4). In particular, exact evaluations have been shown to be analytically tractable in $d=\infty$ [7]. Introducing the functions

$$Y^{(1)}_\sigma(\mathbf{i},\mathbf{j})=\{n_{\mathbf{i}\sigma}n_{\mathbf{j}\sigma}\mathscr{D}\}^{fc}_0, \tag{7a}$$

$$Y^{(2)}_\sigma(\mathbf{i},\mathbf{j})=(g^2-1)\{n_{\mathbf{i}\sigma}D_{\mathbf{j}}\mathscr{D}\}^{fc}_0, \tag{7b}$$

$$Y^{(3)}(\mathbf{i},\mathbf{j})=(g^2-1)^2\{D_{\mathbf{i}}D_{\mathbf{j}}\mathscr{D}\}^{fc}_0, \tag{7c}$$

$$Y^{(4)}_\sigma(\mathbf{i},\mathbf{j})=\{n_{\mathbf{i}\sigma}n_{\mathbf{j}-\sigma}\mathscr{D}\}^{fc}_0 \tag{7d}$$

with [11]

$$Y^{(r)}_{\mathbf{j}}=\frac{1}{2L}\sum_{\mathbf{i},\sigma}Y^{(r)}_\sigma(\mathbf{i},\mathbf{i}+\mathbf{j}) \tag{8}$$

where

$$\mathscr{D}=1+\sum_{m=1}^{\infty}\frac{(g^2-1)^m}{m!}\sum_{\mathbf{f}_1\ldots\mathbf{f}_m}D_{\mathbf{f}_1}\ldots D_{\mathbf{f}_m} \tag{9}$$

the above CFs are determined in terms of the general wave function (4) by

$$C^{SS}_{\mathbf{j}}=2(Y^{(1)}_{\mathbf{j}}-Y^{(4)}_{\mathbf{j}})+\delta_{\mathbf{j},0}[n+2\bar{d}(1-g^2)/g^2]+\frac{1}{L}\sum_{\mathbf{i}}m_{\mathbf{i}}m_{\mathbf{i}+\mathbf{j}}-m^2, \tag{10a}$$

$$C^{NN}_{\mathbf{j}}=2(Y^{(1)}_{\mathbf{j}}+4Y^{(2)}_{\mathbf{j}}+2Y^{(3)}_{\mathbf{j}}+Y^{(4)}_{\mathbf{j}})+\delta_{\mathbf{j},0}[n-2\bar{d}(1-g^2)/g^2]+\frac{1}{L}\sum_{\mathbf{i}}n_{\mathbf{i}}n_{\mathbf{i}+\mathbf{j}}-n^2, \tag{10b}$$

$$C^{ND}_{\mathbf{j}}=2[g^2/(g^2-1)](Y^{(2)}_{\mathbf{j}}+Y^{(3)}_{\mathbf{j}})+\delta_{\mathbf{j},0}2\bar{d}+\frac{1}{L}\sum_{\mathbf{i}}n_{\mathbf{i}}\bar{d}_{\mathbf{i}+\mathbf{j}}-n\bar{d}, \tag{10c}$$

$$C^{DD}_{\mathbf{j}}=[g^2/(g^2-1)]^2Y^{(3)}_{\mathbf{j}}+\delta_{\mathbf{j},0}\bar{d}+\frac{1}{L}\sum_{\mathbf{i}}\bar{d}_{\mathbf{i}}\bar{d}_{\mathbf{i}+\mathbf{j}}-\bar{d}^2. \tag{10d}$$

Here we used $\bar{d}_{\mathbf{i}}=\langle\hat{D}_{\mathbf{i}}\rangle$, $\bar{d}=L^{-1}\sum_{\mathbf{i}}\bar{d}_{\mathbf{i}}$, $n_{\mathbf{i}}=\langle\hat{n}_{\mathbf{i}\uparrow}\rangle+\langle\hat{n}_{\mathbf{i}\downarrow}\rangle$, $n=L^{-1}\sum_{\mathbf{i}}n_{\mathbf{i}}$, $m_{\mathbf{i}}=\langle\hat{n}_{\mathbf{i}\uparrow}\rangle-\langle\hat{n}_{\mathbf{i}\downarrow}\rangle$ and $m=L^{-1}\sum_{\mathbf{i}}m_{\mathbf{i}}$. The curly bracket in (7) indicates the sum over all fully contracted products according to Wick's theorem, as introduced in [9, 10], where contractions have the special property

$$\{c^+_{\mathbf{f}\sigma}c_{\mathbf{h}\sigma}\}_0\equiv\langle\hat{c}^+_{\mathbf{f}\sigma}\hat{c}_{\mathbf{h}\sigma}\rangle_0\equiv P^0_{\sigma,\mathbf{fh}}, \tag{11}$$

$$\{c_{\mathbf{h}\sigma}c^+_{\mathbf{f}\sigma}\}_0\equiv-P^0_{\sigma,\mathbf{fh}} \tag{12}$$

and $\langle\hat{O}\rangle_0\equiv\langle\Phi_0|\hat{O}|\Phi_0\rangle$. In particular, the usual $\delta_{\mathbf{fh}}$ term is missing in (12)! This implies that the objects within $\{\ldots\}_0$ are no longer operators but behave like Grassmann variables. The ensuing simplifications allow for exact evaluations at least in $d=1, \infty$. The superscript "fc" in (7) indicates that only fully-connected graphs are considered, i.e. those where any internal vertex is connected to **i** and **j** by continuous fermion lines [10].

Further simplifications result from introducing a "self-energy" $S_{\sigma,\mathbf{ij}}$, whose diagrams are identical to those in a Green's function approach to a φ^4-theory with lines corresponding to $P^0_{\sigma,\mathbf{ij}}$ [7]. The one-particle density matrix $G_{\sigma,\mathbf{ij}} = \langle \hat{c}^+_{\mathbf{i}\sigma}\hat{c}_{\mathbf{j}\sigma}\rangle$, evaluated in terms of (4), has been derived in [7].

III. Diagrammatic representation of correlation functions

The diagrammatic structure of the functions $Y^{(r)}(\mathbf{i},\mathbf{j})$, (7) which determine the CFs, (6), allows for a compact, coherent representation. To this end we introduce the total four-point vertex function $\Gamma_{\sigma\sigma'}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4})$ via a two-particle quantity $G_{\sigma\sigma'}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4})$ (essentially the two-particle density matrix)

$$G_{\sigma\sigma'}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4}) = -P_{\sigma,\mathbf{13}}P_{\sigma,\mathbf{24}}\delta_{\sigma\sigma'} + P_{\sigma,\mathbf{1}\bar{\mathbf{1}}'}P_{\sigma,\mathbf{2}\bar{\mathbf{2}}'}\Gamma_{\sigma\sigma'}(\bar{\mathbf{1}}',\bar{\mathbf{2}}',\bar{\mathbf{3}}',\bar{\mathbf{4}}')P_{\sigma',\bar{\mathbf{3}}'\mathbf{3}}P_{\sigma',\bar{\mathbf{4}}'\mathbf{4}} \tag{13}$$

where $\mathbf{1}\equiv\mathbf{f}_1$ etc. and variables with a bar are integrated over. Equation (13) is shown diagrammatically in Fig. 1a, with a dressed (fermion) line between two vertices $\mathbf{i},\mathbf{j}$ corresponding to $P_{\sigma,\mathbf{ij}} \equiv \{c^+_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma}\mathcal{D}\}^c_0$. Note that the definitions of $P_{\sigma,\mathbf{ij}}$ and $G_{\sigma,\mathbf{ij}}$ are slightly different [7]. The vertex function $\Gamma_{\sigma\sigma'}$ can be expressed in terms of a two-particle irreducible vertex function $\Gamma^*_{\sigma\sigma'}$ as (see Fig. 1b)

$$\Gamma_{\sigma\sigma'}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4}) = \Gamma^*_{\sigma\sigma'}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4}) - \sum_{\substack{\sigma''=\\ \pm\sigma'}} \Gamma^*_{\sigma\sigma''}(\mathbf{1},\mathbf{2},\bar{\mathbf{3}}',\bar{\mathbf{4}}') \cdot P_{\sigma'',\bar{\mathbf{3}}'\bar{\mathbf{1}}'}P_{\sigma'',\bar{\mathbf{4}}'\bar{\mathbf{2}}'}\Gamma_{\sigma''\sigma'}(\bar{\mathbf{1}}',\bar{\mathbf{2}}',\mathbf{3},\mathbf{4}). \tag{14}$$

The fact that the two external vertices in $Y^{(r)}$ are either connected to two fermion lines each ($Y^{(1)}, Y^{(4)}$), or to two and four lines ($Y^{(2)}$), or to four lines each ($Y^{(3)}$), may be described by a three-point vertex function $\gamma_\sigma(\mathbf{1};\mathbf{2},\mathbf{3})$ where at the external vertex, **1**, four lines merge and where the vertices **2** and **3** are connected to the rest of the diagram by a single line each (see Fig. 1c). Furthermore, there is a trivial vertex

$$\gamma^0(\mathbf{1};\mathbf{2},\mathbf{3}) = \delta_{\mathbf{f}_1\mathbf{f}_2}\delta_{\mathbf{f}_1\mathbf{f}_3}. \tag{15}$$

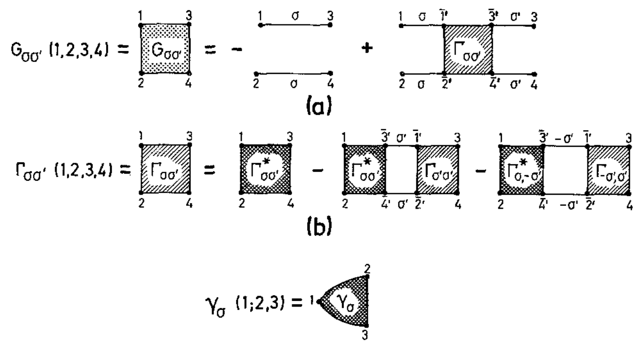

Fig. 1a–c. Diagrammatic representation, (**a**), of (13), expressing the two-particle quantity $G_{\sigma\sigma'}$ in terms of the total four-point vertex function $\Gamma_{\sigma\sigma'}$; (**b**), of (14), expressing $\Gamma_{\sigma\sigma'}$ in terms of the two-particle irreducible vertex function $\Gamma^*_{\sigma\sigma'}$; (**c**), of the three-point vertex function γ_σ

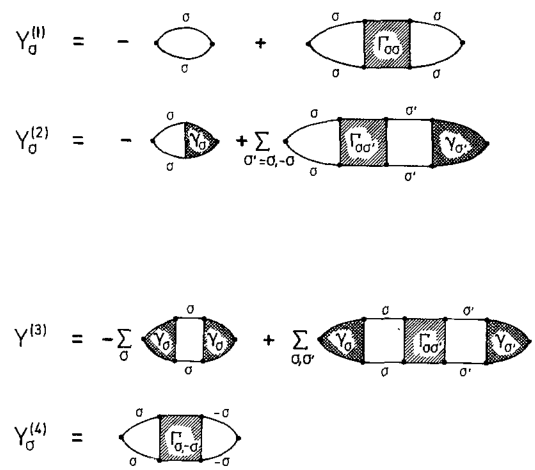

Fig. 2. Diagrammatic representation of (16a–d) for the functions $Y^{(r)}(\mathbf{i},\mathbf{j})$, $r=1,\ldots,4$, which determine the correlation functions, in terms of the vertex functions $\Gamma_{\sigma\sigma'}$ and γ_σ

In this way the functions $Y^{(r)}(\mathbf{f}_1,\mathbf{f}_2)$ are expressed as

$$Y^{(1)}_\sigma(\mathbf{1},\mathbf{2}) = \gamma^0(\mathbf{1};\bar{\mathbf{1}}',\bar{\mathbf{2}}')G_{\sigma\sigma}(\bar{\mathbf{1}}',\bar{\mathbf{2}}',\bar{\mathbf{3}}',\bar{\mathbf{4}}')\gamma^0(\mathbf{2};\bar{\mathbf{3}}',\bar{\mathbf{4}}'), \tag{16a}$$

$$Y^{(2)}_\sigma(\mathbf{1},\mathbf{2}) = \sum_{\substack{\sigma'=\\ \sigma,-\sigma}} \gamma^0(\mathbf{1};\bar{\mathbf{1}}',\bar{\mathbf{2}}')G_{\sigma\sigma'}(\bar{\mathbf{1}}',\bar{\mathbf{2}}',\bar{\mathbf{3}}',\bar{\mathbf{4}}')\gamma_{\sigma'}(\mathbf{2};\bar{\mathbf{3}}',\bar{\mathbf{4}}'), \tag{16b}$$

$$Y^{(3)}(\mathbf{1},\mathbf{2}) = \sum_{\sigma\sigma'} \gamma_\sigma(\mathbf{1};\bar{\mathbf{1}}',\bar{\mathbf{2}}')G_{\sigma\sigma'}(\bar{\mathbf{1}}',\bar{\mathbf{2}}',\bar{\mathbf{3}}',\bar{\mathbf{4}}')\gamma_{\sigma'}(\mathbf{2};\bar{\mathbf{3}}',\bar{\mathbf{4}}') + y^{(3)}(\mathbf{1},\mathbf{2}), \tag{16c}$$

$$Y^{(4)}_\sigma(\mathbf{1},\mathbf{2}) = \gamma^0(\mathbf{1};\bar{\mathbf{1}}',\bar{\mathbf{2}}')G_{\sigma,-\sigma}(\bar{\mathbf{1}}',\bar{\mathbf{2}}',\bar{\mathbf{3}}',\bar{\mathbf{4}}')\gamma^0(\mathbf{2};\bar{\mathbf{3}}',\bar{\mathbf{4}}') \tag{16d}$$

which is shown diagrammatically in Fig. 2. Here $y^{(3)}$ is a diagram where the two external vertices are strictly connected via four lines.

By introducing the above notation the functions $Y^{(r)}$ have been separated diagrammatically into pieces which are two-particle reducible and those which are not. In the former case a diagram can be split into two parts by breaking two lines. On the other hand, external vertices of the irreducible part that do not coincide are always connected by four different paths.

IV. Evaluation in infinite dimensions

In infinite dimensions diagrammatic calculations are greatly simplified by the fundamental property [7]

$$P^0_{\sigma,\mathbf{ij}} \lesssim \mathcal{O}\left(\frac{1}{\sqrt{d}}\right) \quad \text{for } \mathbf{i} \neq \mathbf{j} \tag{17}$$

which implies a collapse of diagrams in which vertices $\mathbf{i}$ and $\mathbf{j}$ are connected by three or more separate paths. This applies directly to the two-particle irreducible vertex functions $\Gamma^*_{\sigma\sigma'}$, γ_σ and to $y^{(3)}$, which therefore reduce to a *single* point vertex

$$\Gamma^*_{\sigma\sigma'}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4}) = \tilde{\Gamma}^*_{\sigma\sigma'}(\mathbf{f}_1)\,\delta_{\mathbf{f}_1\mathbf{f}_2}\delta_{\mathbf{f}_3\mathbf{f}_4}\delta_{\mathbf{f}_1\mathbf{f}_4}, \tag{18a}$$

$$\gamma_\sigma(\mathbf{1};\mathbf{2},\mathbf{3}) = \tilde{\gamma}_\sigma(\mathbf{f}_1)\,\delta_{\mathbf{f}_1\mathbf{f}_2}\delta_{\mathbf{f}_1\mathbf{f}_3}, \tag{18b}$$

$$y^{(3)}(\mathbf{1},\mathbf{2}) = \tilde{y}(\mathbf{f}_1)\,\delta_{\mathbf{f}_1\mathbf{f}_2} \tag{18c}$$

and are thus determined by purely *local* quantities $\tilde{\Gamma}^*_{\sigma\sigma'}(\mathbf{i})$, $\tilde{\gamma}_\sigma(\mathbf{i})$, $\tilde{y}(\mathbf{i})$. Furthermore, (18) implies that the total vertex function $\Gamma_{\sigma\sigma'}$ reduces to

$$\Gamma_{\sigma\sigma'}(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4}) = \tilde{\Gamma}_{\sigma\sigma'}(\mathbf{1},\mathbf{3})\,\delta_{\mathbf{f}_1\mathbf{f}_2}\delta_{\mathbf{f}_3\mathbf{f}_4} \tag{19}$$

where $\tilde{\Gamma}_{\sigma\sigma'}$ obeys the equation

$$\begin{aligned}\tilde{\Gamma}_{\sigma\sigma'}(\mathbf{1},\mathbf{2}) &= \tilde{\Gamma}^*_{\sigma\sigma'}(\mathbf{1})\,\delta_{\mathbf{f}_1\mathbf{f}_2} - \tilde{\Gamma}^*_{\sigma\sigma'}(\mathbf{1})(P_{\sigma',\mathbf{1}\bar{\mathbf{1}}'})^2\,\tilde{\Gamma}_{\sigma'\sigma'}(\bar{\mathbf{1}}',\mathbf{2})\\ &\quad - \tilde{\Gamma}^*_{\sigma-\sigma'}(\mathbf{1})(P_{-\sigma',\mathbf{1}\bar{\mathbf{1}}'})^2\,\tilde{\Gamma}_{-\sigma'\sigma'}(\bar{\mathbf{1}}',\mathbf{2}).\end{aligned} \tag{20}$$

This corresponds to a sum of diagrams consisting entirely of "bubbles" (see the first diagram for $Y^{(1)}_\sigma$ in Fig. 2) made up of dressed σ or $-\sigma$ lines. Equation (20) is valid for $\sigma=\uparrow,\downarrow$ and $\sigma'=\pm\sigma$ and provides a closed system of equations for $\tilde{\Gamma}_{\sigma\sigma}(\mathbf{i},\mathbf{j})$, $\tilde{\Gamma}_{\sigma-\sigma}(\mathbf{i},\mathbf{j}) = \tilde{\Gamma}_{-\sigma\sigma}(\mathbf{i},\mathbf{j})$ and $\tilde{\Gamma}_{-\sigma-\sigma}(\mathbf{i},\mathbf{j})$ in terms of the unknown quantities $\tilde{\Gamma}^*_{\sigma\sigma}(\mathbf{i})$, $\tilde{\Gamma}^*_{\sigma-\sigma}(\mathbf{i})$ and $\tilde{\Gamma}^*_{-\sigma-\sigma}(\mathbf{i})$. Furthermore the three quantities $\tilde{y}(\mathbf{i})$, $\tilde{\gamma}_\sigma(\mathbf{i})$ and $\tilde{\gamma}_{-\sigma}(\mathbf{i})$ have to be determined. This requires six equations for the above six unknowns. They can be obtained from $Y^{(1)}_\sigma(\mathbf{i},\mathbf{i})$ (2 eqs.), $Y^{(2)}_\sigma(\mathbf{i},\mathbf{i})$ (2 eqs.), $Y^{(3)}(\mathbf{i},\mathbf{i})$ (1 equ.) and $Y^{(4)}_\sigma(\mathbf{i},\mathbf{i})$ (1 equ.) which are simple functions of the average electron density and double occupancy $\bar{d}$ at site $\mathbf{i}$; these have been determined earlier [7]. Thereby the problem is formally solved for arbitrary VWFs (4).

In the following we will discuss the explicit results for the Gutzwiller wave function, (5), for $n_\sigma = n_{-\sigma} = n/2$. This case is particularly simple since $|\Psi_G\rangle$ is translationally invariant and symmetric under spin flips. Therefore all six unknown quantities are space-*independent*

$$\tilde{\Gamma}^*_{\sigma\sigma}(\mathbf{i}) = \tilde{\Gamma}^*_{-\sigma-\sigma}(\mathbf{i}) \equiv \Gamma_1, \quad \tilde{\Gamma}^*_{\sigma-\sigma}(\mathbf{i}) = \tilde{\Gamma}^*_{-\sigma\sigma}(\mathbf{i}) \equiv \Gamma_2, \tag{21a}$$

$$\tilde{\gamma}_\sigma(\mathbf{i}) = \tilde{\gamma}_{-\sigma}(\mathbf{i}) \equiv \gamma, \tag{21b}$$

$$\tilde{y}(\mathbf{i}) \equiv y \tag{21c}$$

and $P^0_\sigma(\mathbf{i},\mathbf{i}+\mathbf{j}) \equiv P^0(\mathbf{j})$, $P_\sigma(\mathbf{i},\mathbf{i}+\mathbf{j}) \equiv P(\mathbf{j})$; in the following spin-subscripts will be dropped. In this situation (20) is easy to solve. We define the Fourier transforms of the bubbles $[P(\mathbf{j})]^2$, $[P^0(\mathbf{j})]^2 = [P(\mathbf{j})]^2_{g=1}$, as

$$\Pi(\mathbf{k},n,g) = \sum_{\mathbf{j}} e^{i\mathbf{k}\cdot\mathbf{j}}[P(\mathbf{j})]^2 \tag{22a}$$

and

$$\Pi_0(\mathbf{k},n) = \Pi(\mathbf{k},n,1) = L^{-1}\sum_{\mathbf{k}'} n^0_{\mathbf{k}'} n^0_{\mathbf{k}-\mathbf{k}'} \tag{22b}$$

with $n^0_{\mathbf{k}} = \theta(E_F - \varepsilon_{\mathbf{k}})$, and E_F as the Fermi energy. One finds

$$\Pi(\mathbf{k},n,g) = \left[1 + \frac{1-g^2}{g^2}\,\frac{2\bar{d}}{n}\right]^2 \Pi_0(\mathbf{k},n) \tag{23}$$

where $\bar{d}(n,g)$ is the mean double occupancy of the interacting system. The Fourier transforms of $Y^{(r)}_{\mathbf{j}}$, (8), are then given by

$$Y^{(1)} \pm Y^{(4)} = -\frac{\Pi(\mathbf{k},n,g)}{1 + (\Gamma_1 \pm \Gamma_2)\,\Pi(\mathbf{k},n,g)}, \tag{24a}$$

$$Y^{(2)} = \gamma(Y^{(1)} + Y^{(4)}), \tag{24b}$$

$$Y^{(3)} = y + 2\gamma^2(Y^{(1)} + Y^{(4)}) \tag{24c}$$

where $Y^{(r)} = Y^{(r)}(\mathbf{k},n,g)$. The CFs in momentum space are immediately obtained from (10) by Fouriertransformation ($C^{XY}(\mathbf{k}) = \sum_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{j})\,C^{XY}_{\mathbf{j}}$). The remaining constants Γ_1, Γ_2, y are determined by

$$C^{SS} = C^{NN} = C^{ND} = 0,\; C^{DD} = (g/2)\,\partial\bar{d}/\partial g \equiv p,$$

valid at $\mathbf{k}=0$, where

$$\bar{d} = [-1 + n(1-g^2) + \sqrt{1 - n(2-n)(1-g^2)}]/2(1-g^2)$$

is the density of doubly occupied sites in infinite dimensions (which is identical to the result of the Gutzwiller *approximation*! [7]). The resulting expressions are particularly simple if we introduce the spin/density CFs for the non-interacting case

$$C^{SS}(\mathbf{k}, n, g=1)=C^{NN}(\mathbf{k}, n, g=1)\equiv C_0(\mathbf{k}, n) \tag{25}$$

where $C_0(\mathbf{k}, n)=n-2\Pi_0(\mathbf{k}, n)$. The final result is then given by [12]

$$C^{SS}(\mathbf{k}, n, g)=\frac{C_0(\mathbf{k}, n)}{1-V_s C_0(\mathbf{k}, n)}, \quad V_s=\frac{1}{n-2\bar{d}_0}-\frac{1}{n-2\bar{d}}, \tag{26a}$$

$$C^{NN}(\mathbf{k}, n, g)=\frac{C_0(\mathbf{k}, n)}{1+V_N C_0(\mathbf{k}, n)},$$

$$V_N=\frac{1}{n(1-n)+2\bar{d}}-\frac{1}{n(1-n)+2\bar{d}_0}, \tag{26b}$$

$$C^{ND}(\mathbf{k}, n, g)=q_D C^{NN}(\mathbf{k}, n, g), \quad q_D=\frac{(2-n)\bar{d}}{n(1-n)+2\bar{d}}, \tag{26c}$$

$$C^{DD}(\mathbf{k}, n, g)=p+q_D^2 C^{NN}(\mathbf{k}, n, g) \tag{26d}$$

where $\bar{d}_0=\bar{d}(g=1)=(n/2)^2$. In the atomic limit ($\bar{d}=0$) and for half-filling, C^{NN}, C^{ND}, C^{DD} vanish, while the spin-CF becomes

$$C^{SS}(\mathbf{k}, 1, 0)=\frac{1}{2\Pi_0(\mathbf{k}, 1)}-1. \tag{27}$$

At $\mathbf{k}=\mathbf{Q}=(\pi, \ldots, \pi)$, with $\mathbf{Q}$ as half a reciprocal lattice vector whose magnitude corresponds to $2k_F$, C^{SS} is found to *diverge*. This indicates an antiferromagnetic divergence, the implications of which in position space will be investigated below.

The CFs in $d=\infty$ are seen to have a structure familiar from RPA. This is due to the summation of dressed bubble diagrams, which are the only one to survive in this limit. Hence correlations in $d=\infty$ remain non-trivial only if $\Pi_0(\mathbf{k}, n)$ remains non-trivial (this will be investigated below). The quantities V_S, V_N correspond to renormalized coupling constants. Their simple dependence on n and $\bar{d}$ is not easily obtained from the condition $C^{SS}=0$ etc. at $\mathbf{k}=0$; it is, however, revealed when the Fourier transformation of the CFs into position space is calculated (see below).

In view of the generality of our diagrammatic (but variational) approach to two-particle quantities and the one-to-one correspondence of diagrams obtained thereby to those of a Green's function approach (see the discussion at the end of Sect. II), we expect similar results to be true even for the *exact* solution of the Hubbard model in $d=\infty$. In this limit only bubble-type diagrams consisting of dressed propagators should remain, such that physical quantities (like correlation functions, susceptibilities etc.) will have an RPA-like structure with, however, frequency-dependent vertices, i.e. couplings.

V. The correlation functions in position space

To obtain the CFs in position space, $C_{\mathbf{j}}^{XY}(n, g) = L^{-1}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{j}} C^{XY}(\mathbf{k}, n, g)$, we need to know $\Pi_0(\mathbf{k}, n)$ (written as $\Pi_0(\mathbf{k})$ in short) in $d=\infty$. Making use of the fact that for $d\to\infty$ the density of states (DOS) corresponding to (2) becomes [7]

$$N(E)=\frac{1}{\sqrt{2\pi}\bar{t}} e^{-(E/\bar{t})^2/2} \tag{28}$$

$\Pi_0(\mathbf{k})$ is obtained as (see appendix)

$$\Pi_0(\mathbf{k})=\left(\frac{n}{2}\right)^2-\frac{\bar{t}}{\sqrt{2d}} N^2(E_F)\,\varepsilon_{\mathbf{k}}+\mathcal{O}\left(\frac{1}{d}\right). \tag{29}$$

Hence $\Pi_0(\mathbf{k})$ is essentially given by a *constant* for almost all $\mathbf{k}$, with deviations being small (i.e. of order $1/\sqrt{d}$). Equation (29) suffices to determine the values of the CFs (26) between nearest-neighbors (n.n.).

For example, the $\mathbf{k}$-dependence of the spin-spin CF, (26a), is found from (29) as

$$C^{SS}(\mathbf{k}, n, g)=\frac{n-2\bar{d}_0}{1-V_S(n-2\bar{d}_0)} + \frac{2\bar{t}}{\sqrt{2d}}\frac{N^2(E_F)}{[1-V_S(n-2\bar{d}_0)]^2}\,\varepsilon_{\mathbf{k}}+\mathcal{O}\left(\frac{1}{d}\right) \tag{30}$$

such that in position space it assumes the form

$$C_{\mathbf{j}}^{SS}(n, g)=\frac{n-2\bar{d}_0}{1-V_S(n-2\bar{d}_0)}\,\delta_{\mathbf{j},0} - \frac{\bar{t}^2}{d}\frac{N^2(E_F)}{[1-V_S(n-2\bar{d}_0)]^2}\sum_{i=1}^{d}\delta_{\mathbf{j},\pm\hat{e}_i}+\ldots \tag{31}$$

Here $\{\hat{e}_i\}$ is the d-dimensional set of unit basis-vectors, such that $\{\pm\hat{e}_i\}$ are the n.n. positions to $\mathbf{j}=0$. Higher order corrections in $1/d$ to each one of the first two terms in (31) have been neglected. Similarly, $C_{\mathbf{j}}^{NN}$ is obtained by replacing V_S by $-V_N$. Using $C_{\mathbf{j}=0}^{SS}=n-2\bar{d}$, the renormalized coupling constant is determined as $V_S=(n-2\bar{d}_0)^{-1}-(n-2\bar{d})^{-1}$, thus proving (26a). Hence we find that for n.n. positions $C_{\mathbf{j}}^{SS}$ may be written as

$$C_{\pm\hat{e}_i}^{SS}(n, g)=g_{SS}\,C_{\pm\hat{e}_i}^{SS}(n, g=1) \tag{32a}$$

where

$$g_{SS}(n,g)=\left(\frac{n-2\bar{d}}{n-2\bar{d}_0}\right)^2 \tag{32b}$$

is a renormalization factor with $1\leqq g_{SS}\leqq(1-n/2)^{-2}$. Clearly, g_{SS} describes an *enhancement* of n.n. spin correlations relative to the noninteracting case. We note that this result is identical to that obtained by Zhang, Gros, Rice and Shiba [13] using (semi-)classical counting arguments in the spirit of the Gutzwiller approximation [8, 14]. Indeed, $C^{SS}_{\pm\hat{e}_i}$ is non-zero only if sites $\mathbf{i}$ and $\mathbf{j}=\mathbf{i}\pm\hat{e}_i$ are singly occupied, the average probability for which being given by $\sum_{\sigma\sigma'}(n_{\mathbf{i}\sigma}-\bar{d}_{\mathbf{i}})(n_{\mathbf{j}\sigma'}-\bar{d}_{\mathbf{j}})=(n-2\bar{d})^2$. Hence the enhancement over the non-interacting case is precisely given by (32). This proves once more that in $d=\infty$ the Gutzwiller approximation yields the approximation-free results in terms of the Gutzwiller wave function. In view of this fact it is interesting to note that the numerical evaluations of n.n. spin correlations in terms of (5) in $d=2$ dimensions by Zhang et al. [13] are quantitatively well described by the results (32), valid strictly only in $d=\infty$! The surprising agreement between $d=2$ and $d=\infty$ seems to be due to the dependence of $C^{SS}_{\mathbf{j}}$ on the variational parameter g. In $d=1$ $C^{SS}_{\hat{e}_i}$ for $g=0.2$ is already very close to its limiting value for $g=0$. For such values of g the series expansion in terms of g^2-1 can be terminated after a few terms. At such a low order there are not many diagrams which distinguish between $d=2$ and $d=\infty$, such that the dependence on the dimension d is only weak.

The results for the remaining CFs in (26) have the same structure as (32)

$$C^{XY}_{\pm\hat{e}_i}(n,g)=g_{XY}C^{XY}_{\pm\hat{e}_i}(n,1) \tag{33}$$

where

$$g_{NN}=\left(\frac{n(1-n)+2\bar{d}}{n(1-n)+2\bar{d}_0}\right)^2, \tag{34a}$$

$$g_{ND}=\frac{n(1-n)+2\bar{d}}{n(1-n)+2\bar{d}_0}\,\frac{\bar{d}}{\bar{d}_0}, \tag{34b}$$

$$g_{DD}=\left(\frac{\bar{d}}{\bar{d}_0}\right)^2. \tag{34c}$$

The above renormalization constants have the property $0\leqq g_{XY}\leqq 1$, showing that the deviations in the density and double occupancy from their mean value are reduced by the interaction.

The enhancement of n.n. spin correlations discussed above is only a relative effect. Evidently, a comparison of the first two terms in (31) shows that n.n. spin correlations are actually *small*, of order $1/d$. By contrast, the Néel-state (which is the exact ground state for the Hubbard model in the atomic limit in $d=\infty$ [15]) is rigidly correlated, and the magnitude of correlations does not decrease with distance at all. On this basis we conclude that the simple Gutzwiller wave function, which is an excellent wave function in the atomic limit in $d=1$ [10], is clearly not able to describe spin correlations in high dimensions. A precursor of this feature is already observable in $d=2$ where, according to numerical calculations [16, 17] the magnitude of n.n. spin-CF $\langle\mathbf{S}_{\mathbf{i}}\mathbf{S}_{\mathbf{i}+\hat{e}_i}\rangle$ for $g=0$ is only a little larger than for the Néel state and, in any case, is considerably smaller than the extrapolated exact value. It should be noted that by choosing a more refined starting wave function than the paramagnetic Fermi sea in (4) (e.g. with $|\Phi_0\rangle$ given by antiferromagnetic Hartree-Fock [7] for high dimensions), spin correlations can be constructed to be excellent. However, it is important to note that in this case the semi-classical counting method [13, 18] is no longer applicable in general [7], because it cannot calculate $1/d$-corrections consistently [19].

It should be stressed that the Gutzwiller wave function – although unable to describe spin correlations in high dimensions adequately – does give a correct global description of density-density-correlations, since these are much less subtle than spin correlations.

VI. Beyond nearest neighbor correlations

In view of the shortcomings of the Gutzwiller wave function discussed above, an evaluation of $C^{SS}_{\mathbf{j}}$ beyond n.n. separation of two single spins is by itself not very meaningful. Nonetheless, we note that the correlation between a single spin and a *complete shell* of spins at separation $\mathbf{j}$ is finite even in the limit $d\to\infty$. Making use of this property we will be able to derive a scaling form of this correlation function valid for large spin separations ($|\mathbf{j}|\to\infty$) and strong correlations ($g\to 0$, $n=1$). This will in turn allow us to investigate the functional form of the density of doubly occupied sites $\bar{d}(g)$ for $g\to 0$ in *all* dimensions and thus lead us to the conclusion that the Brinkman-Rice transition only occurs in $d=\infty$ dimensions.

To derive the asymptotic behavior of the correlation between a given spin and a shell of other spins on a hypercubic lattice, we employ the so-called "New

York metric", which measures the distance between a site $\mathbf{j}=(j_1, \ldots, j_d)$ and the origin at $\mathbf{j}=0$ by

$$\|\mathbf{j}\| = \sum_{i=1}^{d} |j_i| \tag{35a}$$

such that

$$\sum_{\mathbf{j}} = \sum_{v=0}^{\infty} \sum_{\|\mathbf{j}\|=v} . \tag{35b}$$

So $\|\mathbf{j}\|$ is determined by going from 0 to $\mathbf{j}$ along the bonds on the square lattice, avoiding diagonal paths. Clearly, there are many different paths of the same length.

In general the CFs in (26) can be written as (here $C^{XY}(\mathbf{k}, n, g) \equiv C^{XY}(\mathbf{k})$)

$$C^{XY}(\mathbf{k}) = \frac{\mu_0 + \mu_1 \Delta\Pi_0(\mathbf{k})}{1 - \mu_2 \Delta\Pi_0(\mathbf{k})} \tag{36}$$

where $\Delta\Pi_0(\mathbf{k}) \equiv \Pi_0(\mathbf{k}, n) - (n/2)^2$ is of the order $(\varepsilon_{\mathbf{k}}/\bar{t})/\sqrt{d}$, i.e. is small for almost all $\mathbf{k}$. The parameters μ_i are easily obtained from (26). Hence (26) may be expanded as

$$C^{XY}(\mathbf{k}) = \sum_{m=0}^{\infty} \lambda_m [\Delta\Pi_0(\mathbf{k})]^m \tag{37}$$

where $\lambda_m = (\mu_0\mu_2 + \mu_1)\mu_2^{m-1}$ for $m \geq 1$ and $\lambda_0 = \mu_0$. In the following we will only consider the spin-spin correlation function; the same analysis also applies to the other CFs.

To calculate $C_{\mathbf{j}}^{XY}$ one has to Fourier transform (37). We make use of the expression for $[P^0(\mathbf{j})]^2$ derived in the appendix for arbitrary $\mathbf{j}$, (A 15). Noting that the dominant contribution to $C_{\mathbf{j}}^{SS}$ is due to $\prod_{l=1}^{d} (\cos k_l)^{|j_l|}$ (see the discussion below (A 11)), and that in the Fourier expansion of $\Delta\Pi_0(\mathbf{k})$ this term appears as $[P^0(\mathbf{j})]^2 \prod_{l=1}^{d} (2\cos k_l)^{|j_l|}$, one obtains

$$C_{\mathbf{j}}^{SS} = \lambda_0 \delta_{\mathbf{j},0} + \sum_{m=1}^{\|\mathbf{j}\|} \lambda_m \sum_{\mathbf{j}^{(1)}, \ldots, \mathbf{j}^{(m)}} \prod_{l=1}^{m} [P^0(\mathbf{j}^{(l)})]^2. \tag{38}$$

Here the second sum is taken over all possible paths from the origin to $\mathbf{j}$ made up of m separate steps $\mathbf{j}^{(l)}$, $l=1, \ldots, m$, with non-negative components [21], such

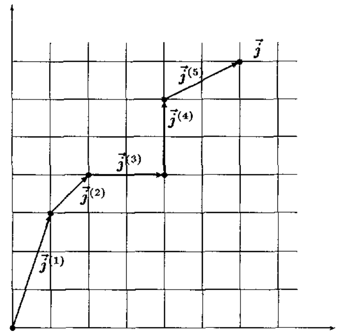

Fig. 3. Example of a typical path connecting the origin and a lattice vector $\mathbf{j}$, which enters in (38). Here the path is composed of $m=5$ steps, each of which is represented by a vector $\mathbf{j}^{(l)}$, $(l=1, \ldots, m)$. The length of $\mathbf{j}^{(l)}$, $\|\mathbf{j}^{(l)}\|$, is measured in the New York metric introduced in (35)

that $\sum_{l=1}^{m} j_i^{(l)} = |j_i|$ (see Fig. 3). For example, for nearest neighbors ($v=1$) one has $\mathbf{j}=\mathbf{j}^{(1)} \equiv \hat{e}_i$ such that $C_{\hat{e}_i}^{SS}$ reduces to (32). In this case n.n. correlations were found to be enhanced when compared with the non-interacting case, the enhancement factor being given by $g_{SS}(n, g) = \lambda_1(n, g)/\lambda_1(n, 1)$. On the other hand, the position vectors of next-nearest neighbors in the New York metric ($v=2$) are given by $\mathbf{j} \equiv \tau_1 = \hat{e}_i + \hat{e}_j$ $(i \neq j)$ and $\mathbf{j} \equiv \tau_2 = 2\hat{e}_i$ for which the spin-CF is found as

$$C_{\tau_1}^{SS} = \lambda_1 [P^0(\hat{e}_i + \hat{e}_j)]^2 + 2\lambda_2 [P^0(\hat{e}_i)]^2 [P^0(\hat{e}_j)]^2 \tag{39}$$

whereas $C_{\tau_2}^{SS}$ is obtained from (39) by $\tau_1 \to \tau_2$, $\hat{e}_j \to \hat{e}_i$ and $2\lambda_2 \to \lambda_2$. Clearly, the correlations between next nearest neighbors (i.e. generally *beyond* nearest neighbors) are now given by a *sum* of terms and are thus not simply renormalized by an overall factor as in the case of n.n. correlations. This shows that semi-classical counting in the spirit of the Gutzwiller-approximation [8, 14] is indeed only valid for n.n. correlations. This is evident from (38), since $C_{\mathbf{j}}^{SS}$ contains contributions from all possible paths of length $\|\mathbf{j}\|$ from the origin to $\mathbf{j}$ covered in m steps. $C_{\mathbf{j}}^{SS}$ is thus determined by the superposition of amplitudes associated with the different steps between sites visited on this route, as is to be expected for a quantum mechanical system. Semi-classical counting methods cannot, in general, estimate these intermediate effects and therefore only apply to n.n. steps.

Since $[P^0(\mathbf{j})]^2$ is small, of order $(1/d)^{\|\mathbf{j}\|}$, the same is true for $C_{\mathbf{j}}^{SS}$ in the case of the Gutzwiller wave function (see (31)). The quantity that does remain finite even for $d \to \infty$ is given by summing over all neighbors at distance $\|\mathbf{j}\|$

$$C_v^{SS} = \sum_{\|\mathbf{j}\|=v} C_{\mathbf{j}}^{SS}. \tag{40}$$

This describes correlations between a given site and a *shell* of sites at distance ν. Expressing the vector $\mathbf{j}$ as a sum of basis vectors $\hat{e}_i$

$$\mathbf{j}=\sum_{m=1}^{\|\mathbf{j}\|} \sigma_{i_m}\hat{e}_{i_m} \tag{41}$$

where $\sigma_i=\pm 1$ and $1 \leqq i_m \leqq d$, we note that for $d\to\infty$ and fixed $\|\mathbf{j}\|$ mere combinatorics implies that nearly all vectors $\mathbf{j}$ with $\|\mathbf{j}\|=\nu$ have ν different values of i_m in (41), i.e. they are made up of ν unit components with the remaining components being zero (e.g. $\mathbf{j}=(1, 1, \ldots, 1, 0, 0, \ldots, 0)$). In this case $\mathbf{j}^2 \simeq \sum_{i=1}^{d} |j_i| = \|\mathbf{j}\| = \nu$. The quantity C_ν^{SS} obeys the required sum rules $C^{SS}(\mathbf{k}=0)=\sum_{\nu=0}^{\infty} C_\nu^{SS}$, and in particular

$$C^{SS}(\mathbf{Q})=\sum_{\nu=0}^{\infty}(-1)^\nu C_\nu^{SS} \tag{42}$$

where $\mathbf{Q}=(\pi, \pi, \ldots, \pi)$ is half a reciprocal lattice vector.

Next, we will determine the asymptotic behavior of C_ν^{SS} for $\nu\to\infty$ in the limit $n=1$ and for strong correlations ($g \ll 1$). This may be extracted from the behavior of $C^{SS}(\mathbf{k})$ at $\mathbf{k}=(1-\delta)\mathbf{Q}$, where a divergence is known to occur at $\delta=0$ (see (27)). For $n=1$ (i.e. $E_F=0$) and $\delta \ll 0$ we find from (A 1), (A 8) and (26.3.1), (26.3.19) of [22] that $\Pi_0[(1-\delta)\mathbf{Q}]=\delta/2$ such that, using (26a),

$$C^{SS}[(1-\delta)\mathbf{Q}]=\frac{1}{\delta+g} \tag{43}$$

for δ, $g \ll 1$. For g fixed, with $\delta \ll g$, we have

$$\Delta C^{SS} \equiv C^{SS}[(1-\delta)\mathbf{Q}]-C^{SS}(\mathbf{Q})=-\frac{\delta}{g^2}+\mathcal{O}(\delta^2). \tag{44}$$

To express $C^{SS}[(1-\delta)\mathbf{Q}]$ in terms of a sum over C_ν^{SS} we write,

$$C^{SS}[(1-\delta)\mathbf{Q}]=\sum_{\mathbf{j}} e^{i(1-\delta)\mathbf{Q}\cdot\mathbf{j}}C_{\mathbf{j}}^{SS} \tag{45a}$$

$$=\sum_{\nu=0}^{\infty}\sum_{\|\mathbf{j}\|=\nu}(-1)^\nu e^{-\frac{1}{2}\pi^2\delta^2\mathbf{j}^2}C_{\mathbf{j}}^{SS} \tag{45b}$$

where the first two factors in (45b) are obtained from the exponential in (45a) in the limit $\delta \ll 1$ and the sum has been converted via (35b). From the discussion below (41) we know that in $d\to\infty$ the sum in (45b) is determined by the vectors $\mathbf{j}$ with $\mathbf{j}^2=\|\mathbf{j}\|$, such that, using (40b),

$$C^{SS}[(1-\delta)\mathbf{Q}]=\sum_{\nu=0}^{\infty}(-1)^\nu\xi^\nu C_\nu^{SS} \tag{46}$$

where $\xi=\cos\delta\pi$, i.e. $\xi^\nu=\exp(-\frac{1}{2}\pi^2\delta^2\nu)$ for small δ. Now we make use of the fact that $(-1)^\nu C_\nu^{SS}\geqq 0$ for $\nu\geqq 0$, (which may be seen from an expansion of (44) in terms of the variable ξ and comparing term by term with (46)) to write

$$(-1)^\nu C_\nu^{SS}=\frac{A(g)}{\nu^\alpha}, \quad \nu\to\infty,\ g\ll 1 \text{ fixed} \tag{47}$$

for the behavior at large ν, where $A(g)$ is a function only of g. Clearly, (47) implies $\Delta C^{SS} \propto A(g)\,\delta^{2(\alpha-1)}$. Comparison with (44) then yields α and $A(g)$ explicitly as

$$C_\nu^{SS}=(-1)^\nu\frac{1}{(2\pi^3)^{1/2}g^2}\frac{1}{\nu^{3/2}}, \quad 1\ll g^{-2}\ll\nu. \tag{48a}$$

By contrast, considering (43) for δ fixed and $g\ll\delta$ and going through the same steps as above one finds

$$C_\nu^{SS}=(-1)^\nu\left(\frac{\pi}{2\nu}\right)^{1/2}, \quad 1\ll\nu\ll g^{-2}. \tag{48b}$$

Hence the limiting behavior of C_ν^{SS} for $\nu\to\infty$ is different depending on whether $\nu\ll g^{-2}$ or $\nu\gg g^{-2}$, the relevant length scale being $1/g^2$.

It is natural to assume that the dependences in (48a), (48b) can be joined smoothly, i.e. that there is a scaling function of the form

$$(-1)^\nu C_\nu^{SS}\propto g^x\varphi(g^y\nu); \quad g\to 0,\ g^y\nu \text{ fixed}. \tag{49}$$

Here $\varphi(z)$ is the inverse Laplace transform of (43), with the limiting behavior $\varphi(z)\propto z^{-1/2}$ for $z\ll 1$ and $\varphi(z)\propto z^{-3/2}$ for $z\gg 1$. This implies $x=1$, $y=2$, such that $(-1)^\nu C_\nu^{SS}\propto g\,\varphi(g^2\nu)$. This also justifies the ansatz made in (47).

VII. Absence of the Brinkman-Rice transition in finite dimensions

The scale dependence of the spin-spin CF in $d=\infty$ determined above is qualitatively identical to that found previously in $d=1$, where [10]

$$C_\nu^{SS}|_{d=1}=\begin{cases}(-1)^\nu\dfrac{1}{\nu}, & 1\ll\nu\ll g^{-2}\\[2ex](-1)^\nu\dfrac{2}{\pi^2}\dfrac{1}{g^2}\dfrac{1}{\nu^2}, & 1\ll g^{-2}\ll\nu\end{cases} \tag{50}$$

(the definition of C_ν^{SS}, (40), is of course also applicable in $d=1$). Only the explicit power of the algebraic decay is seen to be different from that in $d=\infty$. Therefore (50) may equally be expressed by a scaling relation of the form (49), where now $x=y=2$ (note that y is the same as in $d=\infty$) with $\varphi(z)\propto z^{-1}$ for $z\ll 1$ and $\varphi(z)\propto z^{-2}$ for $z\gg 1$.

In view of the striking similarity of the scale dependence of C_ν^{SS} for large ν in the extreme dimensions $d=\infty$ and $d=1$ as given by (48) and (50), respectively, and the existence of a scaling function (49) in both cases, it is natural to assume that a similar behavior is valid also in dimensions $1<d<\infty$. Furthermore we will make a second assumption, namely about the g-dependence of $C^{SS}(\lambda\mathbf{Q})$ at small $|\lambda|$, where $C^{SS}(\lambda\mathbf{Q})\propto|\lambda|$, [23], i.e.

$$C^{SS}(\lambda\mathbf{Q})=f(g)|\lambda|, \quad \lambda\to 0 \tag{51}$$

with $f(\infty)$ *finite* (in $d=1$ and $d=\infty$ $f(g)$ does not even depend on g). To investigate the consequences of the two assumptions we make use of an identity, valid for the Gutzwiller wave function at $n=1$ in arbitrary dimensions

$$C^{SS}[(1-\delta)\mathbf{Q},g]-C^{SS}(\mathbf{Q},g)=-\frac{1}{g^2}\,C^{SS}\left(\delta\mathbf{Q},\frac{1}{g}\right) \tag{52}$$

where [10]

$$C^{SS}(\mathbf{Q},g)=1+2(1-g^2)\frac{\bar{d}}{g^2} \tag{53}$$

which is due to a special particle-hole transformation. Since the l.h.s. of (52) is ΔC^{SS}, defined in (44), application of (51) yields

$$\Delta C^{SS}\simeq-\frac{1}{g^2}f(\infty)|\delta| \quad (\delta\to 0,\ g\ll 1). \tag{54}$$

On the other hand, ΔC^{SS} can independently be determined from (45). To evaluate the sum in (45b) for $d<\infty$ one should note that in this case the length of $\mathbf{j}$ obeys the inequality $\|\mathbf{j}\|/\sqrt{d}\leqq|\mathbf{j}|\leqq\|\mathbf{j}\|$. This implies a very different behavior from that in $d=\infty$, where $|\mathbf{j}|=\sqrt{\|\mathbf{j}\|}$. Namely, for some b with $\pi^2/2d\leqq b\leqq\pi^2/2$, one now has

$$\sum_{\|\mathbf{j}\|=\nu}\exp(-\tfrac{1}{2}\pi^2\delta^2\mathbf{j}^2)\,C_{\mathbf{j}}^{SS}\sim\exp(-b\delta^2\nu^2)\,C_\nu^{SS}. \tag{55}$$

Accordingly, since the sum over ν in (45b) is determined at large ν,

$$\Delta C^{SS}\sim\sum_\nu(-1)^\nu C_\nu^{SS}(\mathrm{e}^{-b\delta^2\nu^2}-1), \tag{56a}$$

$$\propto A(g)|\delta|^{\alpha-1} \tag{56b}$$

where, according to the first assumption, (47) was used, and the sum was replaced by an integral (provided $1<\alpha<3$). Comparison with (54) yields $\alpha=2$ and $A(g)\propto 1/g^2$, such that

$$(-1)^\nu C_\nu^{SS}\propto\frac{1}{g^2}\frac{1}{\nu^2} \quad \nu\to\infty, \quad d<\infty. \tag{57}$$

Hence, for $\nu\to\infty$ one finds the *same* behavior in all dimensions $d<\infty$, which is seen to differ from that in $d=\infty$ (see (48)). This is due to the difference in the form of the majority of vectors $\mathbf{j}$ in $d<\infty$ and $d=\infty$, discussed above.

In the other regime, for large but fixed ν and $g\to 0$, $(-1)^\nu C_\nu^{SS}$ should become independent of g, a behavior parametrized by $(-1)^\nu C_\nu^{SS}\propto 1/\nu^\beta$. We require $\beta\geqq 1/2$ so that correlations in $d<\infty$ are bounded from above by those in $d=\infty$. To join this dependence with that determined in (57) for small but fixed g and $\nu\to\infty$, we employ the scaling form (49). This requires $\varphi(z)\propto 1/z^\beta$ for $z\to 0$ and $\varphi(z)\propto 1/z^2$ for $z\to\infty$, i.e.

$$x=\beta y, \quad x=2(y-1) \tag{58}$$

where $1/2\leqq\beta<2$, i.e. $y\geqq 4/3$. Making use of the dependence of $(-1)^\nu C_\nu^{SS}$ determined above we are now in the position to calculate $C^{SS}(\mathbf{Q},g)$ from (42). Setting this result equal to (53) determines the dependence of $\bar{d}$ on g.

(i) $1<\beta<2$. In this case the sum over $(-1)^\nu C_\nu^{SS}$ converges and yields $C^{SS}(\mathbf{Q},g=0)\sim\mathcal{O}(1)$. From (53) we conclude that $\bar{d}(g)\propto g^\gamma$ with $\gamma\geqq 2$.

(ii) $\beta=1$. Here one finds $C^{SS}(\mathbf{Q},g)\propto\ln(1/g)$ for $g\to 0$, such that $\bar{d}(g)\propto g^2\ln(1/g)$.

(iii) $1/2\leqq\beta<1$ **or** *$4/3\leqq y<2$.* In this case $C^{SS}(\mathbf{Q},g)\propto g^{y-2}$, implying $\bar{d}(g)\propto g^y$.

Thus we find, that in $d<\infty$ dimensions $\bar{d}(g)$ vanishes *faster* than linearly in g for $g\to 0$, such that $\bar{d}(g)/g\to 0$. This is in contrast to the behavior of the kinetic energy at $n=1$ [9], whose expectation value in terms of the Gutzwiller wave function vanishes linearly with g for small g in *all* dimensions $1\leqq d\leqq\infty$. Now, a transition to a localized state with $\bar{d}=0$ at a *finite* interaction strength U ("Brinkman-Rice transition" [20]) occurs only if both terms of the Hubbard-Hamiltonian vanish linearly with g as in the case of $d=\infty$. Introducing $\overline{\varepsilon_0^m}=2L^{-1}\sum_{\mathbf{k}}(\varepsilon_{\mathbf{k}})^m n_{\mathbf{k}}^0$, $\bar{\varepsilon}_0=\overline{\varepsilon_0^1}$, with $\varepsilon_{\mathbf{k}}$ given by (2) and setting

$$E_{\mathrm{kin}}=c_1\bar{\varepsilon}_0 g, \quad \bar{d}=c_2 g \tag{59}$$

minimization of $\langle\hat{H}\rangle/L = E_{\mathrm{kin}} + U\bar{d}$ w.r.t. g determines the critical U as

$$U_c = \frac{c_1}{c_2}\,|\overline{\varepsilon_0}|. \tag{60}$$

In particular, in $d=\infty$ $E_{\mathrm{kin}}^{\infty} = [4g/(1+g^2)]\,\overline{\varepsilon_0}$, $\bar{d}_{\infty} = g/[2(1+g)]$, such that for $g \to 0$ $c_1 = 4$, $c_2 = 1/2$ and $U_c^{\infty} = 8|\overline{\varepsilon_0}|$. Since we found that in $d<\infty$ $\bar{d}(g)$ does not vanish linearly with g we conclude that such a transition does *not* occur at any finite dimension but only at a singular point ($d=\infty$ and $n=1$).

It should be stressed that this finding does not invalidate the general conclusion about the usefulness of the results of the Gutzwiller approximation (i.e. the results for $d=\infty$), which are known to give a very physical description in a number of situations [24–29]. Indeed, as shown by Vollhardt, Wölfle and Anderson [25], the actual transition is unimportant for obtaining a good description of ground state properties of normal liquid ^{3}He.

The question then arises whether the absence of a transition in $d<\infty$ is also obtained within an explicit $1/d$-expansion of the ground state energy. These $1/d$-corrections are obtained diagrammatically if vertices in the diagrams, which are connected by three or more separate paths, are not made to collapse. The contributions of order $1/d$ to E_{kin} and $\bar{d}$ are given by a single diagram each, i.e. $F_{2a}(\mathbf{k})$ and C_{2a} of [9], respectively. For a simple cubic lattice this yields [19]

$$E_{\mathrm{kin}} = E_{\mathrm{kin}}^{\infty}\left[1 - \frac{1}{2d}\left(\frac{1-g}{1+g}\right)^2 \varepsilon_1^2 \varepsilon_2^2 + \mathcal{O}\left(\frac{1}{d^2}\right)\right] \tag{61a}$$

$$\bar{d} = \bar{d}_{\infty}\left[1 - \frac{1}{d}\,\frac{1-g}{(1+g)^2}\,\varepsilon_1^4 + \mathcal{O}\left(\frac{1}{d^2}\right)\right] \tag{61b}$$

where $\varepsilon_1^2 \equiv (\overline{\varepsilon_0}/\bar{t})^2$ and $\varepsilon_2^2 \equiv \overline{\varepsilon_0^2}/\bar{t}^2$. This clearly shows that E_{kin} and $\bar{d}$ remain to be linear in g for small g and that the $1/d$-corrections merely change the coefficients c_1, c_2 in (59). Thereby the critical interaction

$$U_c^{(d)} = U_c^{\infty}\left[1 + \frac{1}{d}\,\varepsilon_1^2\left(\varepsilon_1^2 - \frac{1}{2}\,\varepsilon_2^2\right) + \mathcal{O}\left(\frac{1}{d^2}\right)\right] \tag{62}$$

is shifted to a *larger* value than that in $d=\infty$ (e.g. by about 5% in $d=3$), but is still finite. The above finding indicates that finite orders of perturbation theory in $1/d$ are insufficient to remove the transition. This is not surprising in view of the occurrence of the transition at a singular point as discussed above. In general however, and in particular for more refined wave functions, the limit $d=\infty$ need not be singular. In this case expansions to finite order in $1/d$ around $d=\infty$ may be expected to yield the actual finite-dimensional behavior. This question is presently under investigation.

VIII. Conclusion

In this paper we have formulated a general scheme to calculate correlation functions for lattice electrons in Hubbard-type models in terms of projected wave functions. In this variational approach the Gutzwiller correlation operator, which removes doubly occupied sites in a global fashion, acts on an arbitrary one-particle wave function. As noted before, an explicit evaluation of the diagrammatic contributions is most simple in $d=\infty$. In this limit only diagrams composed of dressed bubbles survive, which may be summed explicitly. This leads to a RPA-type structure of all correlation functions. In view of the generality of our approach we expect that this result holds even in the case of a general Green's function approach to the Hubbard-model in $d=\infty$ [31]. Hence we expect that diagrams with this structure determine the correlations even in the *exact* solution of the model in $d=\infty$.

Explicit, analytic evaluations were performed using the simple Gutzwiller wave function. We found that nearest neighbor correlations in the interacting case are given by the non-interacting result multiplied by an overall renormalization factor. In particular, in the case of the spin-spin correlation function one obtains an enhancement, which is identical to that derived earlier by Zhang et al. [13] using semi-classical counting arguments in the spirit of the Gutzwiller approximation [8, 14]. However, correlations beyond nearest neighbors are seen to be more complicated and cannot be obtained by simple counting. By calculating the absolute value of nearest neighbor spin-correlations we found that these are actually only of the order of $1/d$, i.e. vanishingly small in high dimensions. Consequently, the Gutzwiller wave function leads to grossly inadequate spin-correlations in high dimensions.

Exploiting the fact that correlations between a single spin and a complete shell of other spins remain finite, the asymptotic behavior of the spin-correlation function for large separations was calculated. Its qualitative behavior was found to be very similar to that in $d=1$ and to obey the same scaling form. Assuming this form to hold in all dimensions $1<d<\infty$, too, the functional dependence of $\bar{d}$, the density of doubly occupied sites, on g was inferred. From this it followed that a Brinkman-Rice transition [20], i.e. a transition to a localized state at finite interaction, does not occur in any finite dimension but only at $d=\infty$, i.e. at a singular point. Indeed, finite orders of perturbation theory in $1/d$ do not remove the transition. On the other hand, for more general variational wave functions than the simple Gutzwiller wave functions, $1/d$ expansions should well be applicable. A clarification of this question will certainly also be relevant for a Green's function approach to the Hubbard-model [31] and related models [12, 32] in high dimensions. These will be investigated in future work.

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Appendix: Calculation of $\Pi_0(\mathbf{k})$

The non-interacting bubble $\Pi_0(\mathbf{k})$, (22b), may be interpreted as the joint probability that $\varepsilon_{\mathbf{k}'}, \varepsilon_{\mathbf{k}-\mathbf{k}'} \leqq E_F$ for a randomly chosen vector $\mathbf{k}'$ from the first Brillouin zone (1.BZ). Here $\varepsilon_{\mathbf{k}}$ is the energy dispersion (2). Hence we write

$$\Pi_0(\mathbf{k}) = \int_{-\infty}^{E_F} \mathrm{d}E_1 \int_{-\infty}^{E_F} \mathrm{d}E_2 N_{\mathbf{k}}(E_1, E_2) \tag{A1}$$

where

$$N_{\mathbf{k}}(E_1, E_2) = \frac{1}{(2\pi)^d} \iint_{1.\mathrm{BZ}} \mathrm{d}\mathbf{k}_1 d\mathbf{k}_2 \delta(E_1 - \varepsilon_{\mathbf{k}_1}) \delta(E_2 - \varepsilon_{\mathbf{k}_2}) \cdot \delta^*(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}) \tag{A2}$$

is the probability density for $\varepsilon_{\mathbf{k}_1} = E_1$, $\varepsilon_{\mathbf{k}-\mathbf{k}_1} = E_2$ for given $\mathbf{k}$. $\delta^*(\mathbf{k}) = \sum_{\mathbf{j}} \exp(\mathrm{i}\mathbf{k}\cdot\mathbf{j})$ is the Laue-function, which gives momentum conservation up to a reciprocal lattice vector. The transform of $N_{\mathbf{k}}$

$$G_{\mathbf{k}}(\tau_1, \tau_2) = \int \mathrm{d}E_1 \int \mathrm{d}E_2 N_{\mathbf{k}}(E_1, E_2) \mathrm{e}^{\mathrm{i}E_1\tau_1} \mathrm{e}^{\mathrm{i}E_2\tau_2} \tag{A3}$$

is then obtained from (A1) by using (9.1.21) of [22] and (57.20.3) of [30], as

$$G_{\mathbf{k}}(\tau_1, \tau_2) = \prod_{l=1}^{d} J_0(x_l) \tag{A4}$$

where $J_0(z)$ is the Bessel function of order $n=0$ and

$$x_l = \sqrt{\frac{2}{d}}\, \bar{t}[\tau_1^2 + \tau_2^2 + 2\tau_1\tau_2 \cos k_l]^{1/2}. \tag{A5}$$

Equation (A4) is valid for all dimensions d. For $d \to \infty$ x_l is small for all l. Expanding about $x_l = 0$ up to x_l^2 then yields

$$G_{\mathbf{k}}(\tau_1, \tau_2) = \exp\left[-\frac{1}{2}\tau \cdot \tilde{a} \cdot \tau + \mathcal{O}\left(\frac{1}{d}\right)\right] \tag{A6}$$

where $\tau = (\tau_1, \tau_2)$ and

$$\tilde{a} = \bar{t}^2 \begin{pmatrix} 1 & \tilde{\varepsilon}_{\mathbf{k}} \\ \tilde{\varepsilon}_{\mathbf{k}} & 1 \end{pmatrix} \tag{A7}$$

with $\tilde{\varepsilon}_{\mathbf{k}} = -\varepsilon_{\mathbf{k}}/[\bar{t}\sqrt{2d}]$. Note, that $\tilde{\varepsilon}_{\mathbf{k}}$ is small for general (i.e. almost all) $\mathbf{k}$. To leading order in d, $G_{\mathbf{k}}$ is seen to have a Gaussian form [33], which may be inverted to yield

$$N_{\mathbf{k}}(E_1, E_2) = \frac{1}{2\pi} \frac{1}{\sqrt{\det \tilde{a}}} \exp\left[-\frac{1}{2} \mathbf{E} \cdot (\tilde{a})^{-1} \cdot \mathbf{E}\right] \tag{A8}$$

where $\mathbf{E} = (E_1, E_2)$. For $d \to \infty$ and a general value of $\mathbf{k}$ one has $\mathbf{E} \cdot (\tilde{a})^{-1} \cdot \mathbf{E} \simeq (E_1^2 + E_2^2)/\bar{t}^2$, such that $N_{\mathbf{k}}(E_1, E_2)$ is simply the product of the DOS (28) at $E = E_1$ and $E = E_2$. In this case E_1 and E_2 are *independent*, random variables. Their relative dependence only enters to order $1/\sqrt{d}$ via the off-diagonal term of (A8). $\Pi_0(\mathbf{k})$ is then found as

$$\Pi_0(\mathbf{k}) = \left(\frac{n}{2}\right)^2 - \frac{\bar{t}}{\sqrt{2d}} N^2(E_F)\varepsilon_{\mathbf{k}} + \mathcal{O}\left(\frac{1}{d}\right) \tag{A9}$$

and $[P^0(\mathbf{j})]^2$ for $\|\mathbf{j}\| \leqq 1$ is immediately obtained by Fourier transform. It should be noted that for *special* values of $\mathbf{k}$ (e.g. $\mathbf{k} = 0$) $\Pi_0(\mathbf{k})$ deviates significantly from the average value $(n/2)^2$. This is indeed necessary for relations such as $\Pi_0(\mathbf{k} = 0) = n/2$ to be fulfilled, but it is irrelevant for the overall behavior of $\Pi_0(\mathbf{k})$ since this only occurs at isolated points.

The values of $[P^0(\mathbf{j})]^2$ for $\mathbf{j}$ beyond nearest neighbor separation to $\mathbf{j} = 0$ cannot be calculated from (A8) or (A9) since this requires one to include higher orders than x_l^2 in the expansion of $J_0(x_l)$. Using the expansion (see Eq. (9.1.10) of [22])

$$J_0(x_l) = \sum_{n=0}^{\infty} \frac{1}{(n!)^2} \left(-\frac{1}{4} x_l^2\right)^n \tag{A10a}$$

$$= J_0(\sqrt{y_0}) \sum_{n=0}^{\infty} b_n(y_0)\, y_l^n \tag{A10b}$$

where $y_0=(2\bar{t}^2/d)(\tau_1^2+\tau_2^2)$, $y_l=(4\bar{t}^2/d)\tau_1\tau_2\cos k_l$, and the coefficients b_n are given by

$$b_n(y_0)=[n!J_0(\sqrt{y_0})]^{-1}\sum_{m=0}^{\infty}\left(-\frac{1}{4}\right)^{m+n}\frac{y_0^m}{m!(m+n)!}. \tag{A 11}$$

Furthermore, we introduce the transform

$$\rho_{\mathbf{j}}(E_1,E_2)=\frac{1}{(2\pi)^d}\int_{1.\mathrm{BZ}}\mathrm{d}\mathbf{k}\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{j}}N_{\mathbf{k}}(E_1,E_2). \tag{A 12}$$

The dominant contribution to $[P^0(\mathbf{j})]^2$ for $d\to\infty$ is due to the term proportional to $\prod_{l=1}^{d}(y_l)^{|j_l|}$ in (A4). Transforming from τ_1, τ_2 and $\mathbf{k}$ to E_1, E_2 and $\mathbf{j}$, one obtains

$$\rho_{\mathbf{j}}(E_1,E_2)=\left(-\frac{\bar{t}^2}{2d}\right)^{\nu}\frac{F_\nu(E_1)F_\nu(E_2)}{[\Pi_{i=1}^{d}|j_i|!]^2} \tag{A 13}$$

where the distance $\nu=\|\mathbf{j}\|$ is measured in the New York metric (see (35a)) and

$$F_\nu(E)=\frac{1}{2\pi}\int\mathrm{d}\tau\,\mathrm{e}^{-\mathrm{i}E\tau}\tau^\nu\mathrm{e}^{-\frac{1}{2}\bar{t}^2\tau^2} \tag{A 14a}$$

$$=i^\nu N^{(\nu)}(E) \tag{A 14b}$$

with $N^{(\nu)}(E)=d^\nu N(E)/dE^\nu$ as the ν-th derivative of the DOS, (28). From (A 1) we then obtain the final result

$$[P^0(\mathbf{j})]^2=\left[\frac{N^{(\nu-1)}(E_F)}{\Pi_{i=1}^{d}|j_i|!}\right]^2\left(\frac{\bar{t}^2}{2d}\right)^{\nu}. \tag{A 15}$$

We note that, apart from a combinatorial factor, the $\mathbf{j}$-dependence of $[P^0(\mathbf{j})]^2$ is entirely contained in $\|\mathbf{j}\|$. If we define $N^{(-1)}(E)\equiv n/2$, (A 15) even holds for $\mathbf{j}=0$.

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P.G.J. van Dongen, F. Gebhard, D. Vollhardt
Institut für Theoretische Physik C
Technische Hochschule Aachen
Erweiterungsgelände Seffent-Melaten
D-5100 Aachen
Federal Republic of Germany