



ELSEVIER

Physics Letters A 277 (2000) 35–41

PHYSICS LETTERS A

www.elsevier.nl/locate/pla

Cluster expansion of the many-body Green operator

J. Berakdar

Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

Received 8 September 2000; received in revised form 16 October 2000; accepted 16 October 2000

Communicated by B. Fricke

Abstract

A scheme is presented for expressing the many-body Green operator of an interacting system in terms of Green operators of systems with a fewer number of interacting particles. The method relies on an exact algebraic operator identity proved in this work. Furthermore, we present a hierarchical approximation that reduces successively the many-body problem to a lower dimensional solvable problem. Recipes for higher order corrections are given and practical applications are pointed out. © 2000 Elsevier Science B.V. All rights reserved.

In recent years there has been an impressive progress in computational material science [1]. This development is driven by the unprecedented growth of computational resources and by the demand for yet more precise information on technologically relevant material properties, such as the optical, transport and magnetic characteristics. On the microscopic level, those properties can be obtained from the eigensolutions of the many-body quantum Hamiltonian of the system under study. Thus, one has to deal with the notoriously difficult many-body problem in a computationally acceptable manner. For this purpose remarkably successful and efficient conceptual schemes have been developed where the multi-particle system is mapped onto a one body problem for a particle moving in an effective (non-local) field created by all the other constituents of the system [2,3]. Usually, this effective field is further simplified according to certain recipes such as those provided by the local approximation within the density functional theory [4]. It is these theoretical concepts that rendered possible the calculation of the behavior of many particle systems. A wealth of static properties, such as the ground state energies are well described by such effective one particle methods for a considerable number of elements. However, static features of strongly correlated systems, such as transition metal oxides, still pose a challenge to single particle theories [3]. In addition, for the theoretical description of the many-body excitation spectrum [6] and for the treatment of dynamical processes, such as many particle reactive scattering, methods have to be envisaged that go beyond the single particle picture.

For example, correlated many-body states are a prerequisite for the theoretical formulation of recent measurements of the double and triple electronic excitation of localized or delocalized electronic compounds by one ultraviolet photon [5,7,8]. Recent technological advances have made it even possible to explore in full details the many-body continuum spectrum of four and more interacting particles [8–13] where numerical calculations are absent. Thus, it is desirable to develop, for many-body interacting systems, conceptually sound methods and schemes of approximations that can be numerically implemented.

E-mail address: jber@mpi-halle.de (J. Berakdar).

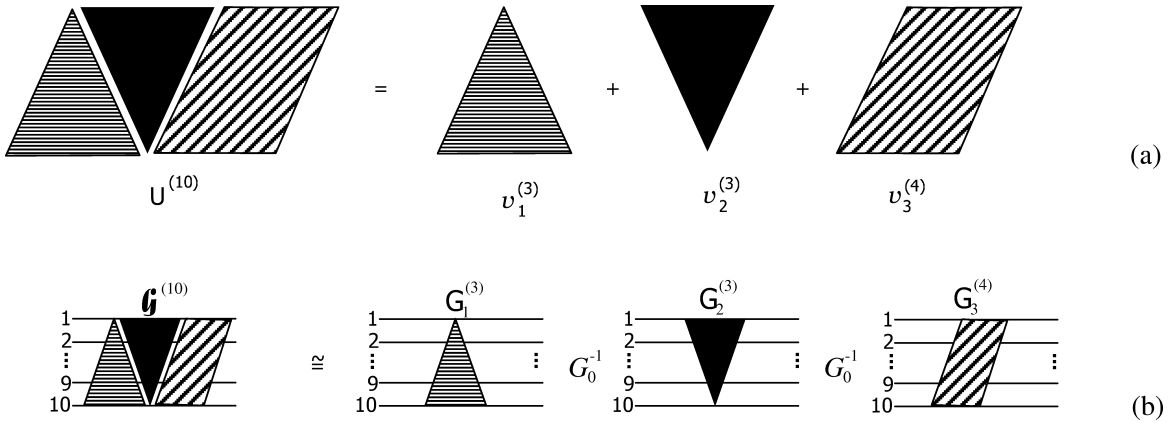


Fig. 1. (a) A pictorial representation of the potential decomposition (1) for a system consisting of three clusters. The coupled particles are located at the corners of the geometrical shapes. Thus, two of the clusters contain three interacting particles each, whereas one cluster encompasses four coupled particles. The shading of the shapes indicates that the various clusters might have different inherent internal dynamics. (b) A diagrammatic illustration of the Green operator expansion (16) which corresponds to the decomposition in (a). Each of the diagrams stands for a Green operator (written above it) with an interaction symbolized by the geometrical shapes (explained in (a)). The particles are indicated by straight lines.

In this study we design for an interacting many-body system a theoretical framework, within which the many-body state is derived cumulatively from the solution of a lower dimensional problem. To deal with strongly correlated systems, the treatment should not give a preference to a certain interaction. Furthermore, the method provides a systematic and mathematically sound scheme for approximations that are computationally manageable and allows, when desirable, to incorporate well established single particle and perturbative approaches.

The fundamental quantity that describes the behavior of the quantum N body system is the total Green operator $\mathcal{G}^{(N)}$ which is the resolvent of the respective Hamiltonian. Our goal is thus to find exact expressions for $\mathcal{G}^{(N)}$ in terms of quantities of lower dimensionality that are computationally accessible. To this end we consider two distinct cases.

Case 1. The N -body system can be broken down into L clusters. The cluster labeled by the number l contains m_l coupled particles. Thus, we require $\sum_l^L m_l = N$. The m_l particles within each subdivision are interacting via the potential $v_l^{(m_l)}$ so that the total interaction $U^{(N)}$ can be cast in the form

$$U^{(N)} = \sum_l^L v_l^{(m_l)}. \quad (1)$$

The non-relativistic total Hamiltonian of the system can be written as $H^{(N)} = K + U^{(N)}$, where K is the kinetic energy operator. Fig. 1(a) demonstrates geometrical decomposition (1).

Let us introduce the Green operator \mathcal{G}_m of a system with the total potential $\sum_{j=1}^m v_j^{(m_j)}$, $m \in [1, L]$. Thus, $\mathcal{G}_L \equiv \mathcal{G}^{(N)}$, where $\mathcal{G}^{(N)}$ is the Green operator of the total system. As

$$H^{(N)} = \left(K + \sum_{j=1}^{m-1} v_j^{(m_j)} \right) + \sum_{j=m}^L v_j^{(m_j)}$$

we can treat G_{m-1} as a reference Green operator and deduce from the Lippmann–Schwinger equation the recurrence relations

$$G^{(N)} \equiv G_L = G_{L-1}[\mathbf{1} + v_L^{(mL)} G_L], \tag{2}$$

$$G_{L-1} = G_{L-2}[\mathbf{1} + v_{L-1}^{(mL-1)} G_{L-1}]. \tag{3}$$

These equations are reformulated in the simple but exact product expansion

$$G^{(N)} = \prod_{j=1}^{L-1} [\tilde{G}_j G_0^{-1} \tilde{G}_{j+1}], \tag{4}$$

where

$$\tilde{G}_j = G_0 + G_0 v_j^{(mj)} G_j. \tag{5}$$

Expansion (4) is derived for a system that can be naturally subdivided into clusters each of which possesses a characteristic internal dynamical structure (dictated by the terms in Eq. (1)). The total Green operator of the system is constructed from the Green operators of the individual clusters by means of Eq. (4). Here the question arises whether it is possible to perform similar analysis to systems that are completely coupled entities, such as the individual clusters themselves. The answer to this question leads us to the second case.

Case 2. We consider a strongly interacting finite system consisting of n particles. We attempt at expressing the many-body Green operator $G^{(n)}$ in terms of lower dimensional Green operators. For the further development we need assume a certain class for the interaction potentials. In what follows we treat the case where the total potential is of the form $U^{(n)} = \sum_{j>i=1}^n v_{ij}$, where v_{ij} have not to be further specified. The method can be generalized to more than two body interactions in a straightforward manner. The total potential $U^{(n)}$ can be decomposed as

$$U^{(n)} = \sum_{j=1}^n u_j^{(n-1)}, \tag{6}$$

$$u_j^{(n-1)} = \sum_{k=1}^{n-1} u_k^{(n-2)}, \quad j \neq k, \tag{7}$$

where $u_j^{(n-1)} = \tilde{u}_j^{(n-1)} / (n-2)$. Here $\tilde{u}_j^{(n-1)}$ is the total potential of a system consisting of $n-1$ interacting particles while the particle j is free (“disconnected”). In terms of the two-body interactions (v_{mn}) the collective potential $\tilde{u}_j^{(n-1)}$ is expressed as $\tilde{u}_j^{(n-1)} = \sum_{r>s=1}^n v_{rs}$, $r \neq j \neq s$. In Fig. 2(a) expansion (6) is explained geometrically.

The basic idea behind the exact relation (6) is to divide the completely interacting system into coupled clusters [cf. Eqs. (1), (6)] with an internal interaction.

Now, let us introduce the Green operator $G_m^{(n-1)}$ of a system with the total potential (sum of collective potentials) $\sum_{j=1}^m u_j^{(n-1)}$, $m \in [1, n]$ (note $G_n^{(n-1)} \equiv G^{(n)}$). As

$$H^{(n)} = \left(K + \sum_{j=1}^{m-1} u_j^{(n-1)} \right) + \sum_{j=m}^n u_j^{(n-1)}$$

we consider $G_{m-1}^{(n-1)}$ as a reference and conclude the recurrence relations

$$G^{(n)} = G_{n-1}^{(n-1)}[\mathbf{1} + u_n^{(n-1)} G_n^{(n-1)}], \tag{8}$$

$$G_{n-1}^{(n-1)} = G_{n-2}^{(n-1)}[\mathbf{1} + u_{n-1}^{(n-1)} G_{n-1}^{(n-1)}]. \tag{9}$$

Again, these equations can be compactly written in the form

$$G^{(n)} = \prod_{j=1}^{n-1} [\tilde{G}_j^{(n-1)} G_0^{-1} \tilde{G}_{j+1}^{(n-1)}], \quad (10)$$

where

$$\tilde{G}_j^{(n-1)} = G_0 + G_0 u_j^{(n-1)} G_j^{(n-1)}. \quad (11)$$

At first sight it seems that little has been gained by the above mathematical manipulation, since on the right-hand side of Eqs. (4), (10) the total Green operator appears. However, the following theorem can be shown (through lengthy but otherwise exact operator algebra):

Let $G_l^{(k)}$, $k, l \in [2, n]$, be the Green operator of a system with k interacting particles subject to the potential $\sum_{j=1}^l u_j^{(k)}$. The Green operator $G_l^{(k)}$ can be written in the form $G_l^{(k)} = G_0 + \sum_{j=1}^l \Gamma_j^{(k)}$. The operators $\Gamma_j^{(k)}$ are related to the Green operators $g_j^{(k)}$ of the systems in which the k particles are correlated by virtue of $u_j^{(n-1)}$ via the linear coupled integral equation

$$\begin{pmatrix} \Gamma_1^{(k)} \\ \Gamma_2^{(k)} \\ \vdots \\ \Gamma_{l-1}^{(k)} \\ \Gamma_l^{(k)} \end{pmatrix} = \begin{pmatrix} g_1^{(k)} - G_0 \\ g_2^{(k)} - G_0 \\ \vdots \\ g_{l-1}^{(k)} - G_0 \\ g_l^{(k)} - G_0 \end{pmatrix} + [\mathbf{K}^{(k)}] \begin{pmatrix} \Gamma_1^{(k)} \\ \Gamma_2^{(k)} \\ \vdots \\ \Gamma_{l-1}^{(k)} \\ \Gamma_l^{(k)} \end{pmatrix}. \quad (12)$$

The kernel $[\mathbf{K}^{(k)}]$ contains only Green operators with a reduced number of interactions and is given by

$$[\mathbf{K}^{(k)}] = \begin{pmatrix} 0 & g_1^{(k)} - G_0 & g_1^{(k)} - G_0 & \dots & g_1^{(k)} - G_0 \\ g_2^{(k)} - G_0 & 0 & g_2^{(k)} - G_0 & \dots & g_2^{(k)} - G_0 \\ \dots & \dots & \dots & \dots & \dots \\ g_{l-1}^{(k)} - G_0 & \dots & g_{l-1}^{(k)} - G_0 & 0 & g_{l-1}^{(k)} - G_0 \\ g_l^{(k)} - G_0 & \dots & g_l^{(k)} - G_0 & g_l^{(k)} - G_0 & 0 \end{pmatrix} G_0^{-1}. \quad (13)$$

It can be further shown that the kernel $[\mathbf{K}^{(k)}]$ is square integrable (i.e., the norm $\|[\mathbf{K}^{(k)}]\| = [\text{Tr}([\mathbf{K}^{(k)}][\mathbf{K}^{(k)}]^\dagger)]^{1/2}$ is square integrable). Therefore, Eq. (12) can be solved by standard methods for treating integral equations of the Fredholm type. Here we just consider the first term (iteration) of Eq. (12) from which we deduce

$$G_l^{(k)} = G_0 + \sum_{j=1}^l g_j^{(k)} - l G_0. \quad (14)$$

The central quantity in Eqs. (4), (10) is of the form $G_0 + G_0 u_l^{(k)} G_l^{(k)}$. From Eq. (14) we conclude that

$$\begin{aligned} G_0 + G_0 u_l^{(k)} G_l^{(k)} &= G_0 + G_0 u_l^{(k)} g_l^{(k)} + G_0 u_l^{(k)} g_{l-1}^{(k)} + \dots + G_0 u_l^{(k)} g_1^{(k)} - (l-1) G_0 u_l^{(k)} G_0 \\ &= g_l^{(k)} + G_0 u_l^{(k)} (G_0 + G_0 u_{l-1}^{(k)} g_{l-1}^{(k)}) + \dots + G_0 u_l^{(k)} (G_0 + G_0 u_1^{(k)} g_1^{(k)}) - (l-1) G_0 u_l^{(k)} G_0 \\ &= g_l^{(k)} + G_0 u_l^{(k)} (G_0 u_{l-1}^{(k)} g_{l-1}^{(k)} + \dots + G_0 u_1^{(k)} g_1^{(k)}). \end{aligned} \quad (15)$$

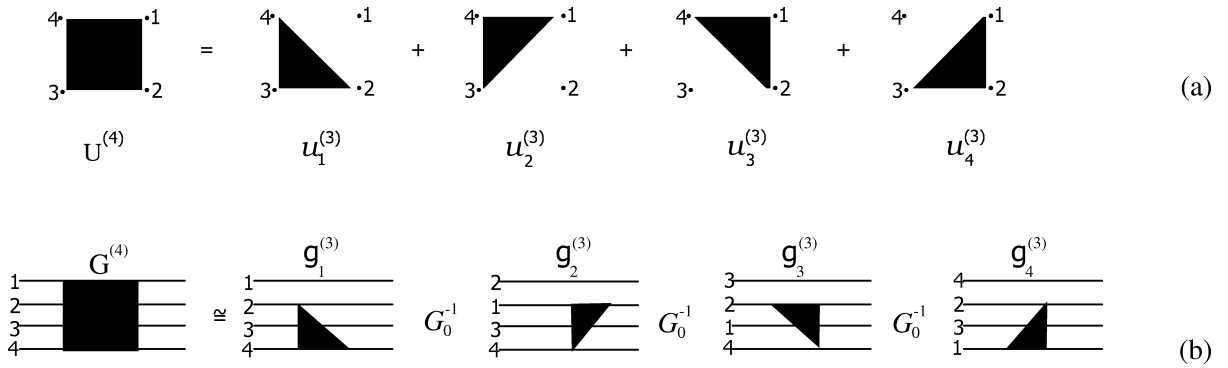


Fig. 2. (a) The reduction of a four interacting particle potential (indicated by a square) to a sum of three body potentials (depicted as triangles) according to Eq. (6). The interacting particles are located at the corners of the geometrical shapes. The orientation of the triangles signifies which particles are interacting. (b) According to Eq. (17), the interaction decomposition shown in (a) leads to a product expansion of the total Green operator in terms of Green operators with a reduced number of interacting particles. Each of the diagrams stands for the Green operator (indicated above it) that involves the interaction symbolized by the geometric shape. The particles are shown as straight lines. Only particles are interacting whose lines cross a triangle.

The leading term of Eq. (15) is identified as the Green operator $g_l^{(k)}$. All other terms are higher order multiple scattering between different subdivisions of the total system. Hence the first order terms in the exact expansions (4) and (10) attain respectively the forms

$$G^{(N)} \stackrel{1\text{-order}}{\equiv} \prod_{j=1}^{L-1} G_j^{(m_j)} G_0^{-1} G_{j+1}^{(m_{j+1})} \tag{16}$$

and

$$G^{(n)} \stackrel{1\text{-order}}{\equiv} \prod_{j=1}^{n-1} g_j^{(n-1)} G_0^{-1} g_{j+1}^{(n-1)}, \tag{17}$$

$$g_j^{(n-1)} \stackrel{1\text{-order}}{\equiv} \prod_{l=1}^{n-2} g_l^{(n-2)} G_0^{-1} g_{l+1}^{(n-2)}, \quad l \neq j. \tag{18}$$

In Eq. (16) only the Green operators $G_j^{(m_j)}$ of the individual (isolated) clusters occur. Fig. 1(b) illustrates expansion (16) for the potential decomposition shown in Fig. 1(a). Note, that since each cluster j contains m_j interacting particles, $G_j^{(m_j)}$ is in fact a correlated m_j particle Green operator. A recipe to deal with such interacting many-body Green operators is provided by Eqs. (17), (18) which allow to deduce the Green operator of a system of n interacting particles in a cumulative way from Green operators with a reduced dimensionality (lower number of interactions). An example is shown diagrammatically in Fig. 2(b) for the corresponding situation of Fig. 2(a). The correction terms beyond approximation (17), (18) are readily given by Eq. (15). It should be noted here that for the case of a three interacting particle system the present results coincide with those obtained in Ref. [15].

The validity of the approximate expressions (17), (18) relies on the truncation of the multiple scattering series Eq. (15) after the first term. This first order approximation means that, within each individual cluster, multiple scattering events are taken into account to all order via g_l^k . However, scattering between various clusters is neglected. For example, in the three-body Coulomb case g_l^k in Eq. (15) is a two-body Green operator (known analytically). Eq. (17) accounts then for two-body interactions but excludes three-body ones which are of a

shorter range (cf., e.g., second term of Eq. (15)). This is a first hint that the present proposal for approximation is reasonable, when for a particular physical system processes involving u_l^k are more important than those mediated by $u_l^k u_{l-1}^k$. Thus, the present method is not appropriate for the special case of zero-range potentials.

For practical application we operate as follows: The first step is to envisage whether the system can be separated in individual clusters as given by Eq. (1). If yes, we use Eq. (16) to deduce the total Green operator. The Green operators of the individual clusters with interacting m_l particle can then be deduced according to Eqs. (17), (18). If a solution of the m_l body problem is not possible we can reduce it to the $m_l - k$ problem using Eqs. (17), (18) for which the solution can be found, e.g., from other analytical or numerical procedures or from an effective field method. Thus, the method shown here is quite flexible and can be employed as a basis for a family of solutions.

Finally, the following general features should be noted: (1) Usually, the various Green operators of the reduced systems can be derived only approximately. The product expansions (16)–(18) have the advantage that no spurious interference terms can occur due to different approximate treatment of the various reduced systems. (2) It is decisive to realize that relations (17), (18) are expansions in the number of *interactions* and not in the number of *particles*. The number of particles in each of the clusters is the same. It is only the number of *interacting* particles in the individual clusters which is reduced (with respect to the total number of interactions). Because of this the symmetry of a (fermionic, bosonic) system can be taken into account when calculating the desired observables from the Green operator. For example, the spectral function can be extracted from the trace of the imaginary part of $G^{(n)}$. The symmetry of the system enters then through the appropriate symmetry of the states used to obtain the trace of $G^{(n)}$. (3) Eqs. (4), (10) are algebraic operator identities and are valid for all abstract operators. Thus, the theory is readily applied to atomic, molecular, nuclear, and condensed matter systems [14]. (4) For many interacting particles $n \geq 3$ the Lippmann–Schwinger equations do not provide unique state vectors [16] and their kernel is not square integrable (and also not compact) [17]. As shown by Faddeev [17] the reason for this shortcoming is the occurrence of the so-called disconnected diagrams where one of the n particles is not interacting, i.e., not correlated with the other $n - 1$ particles. For the present case it can be shown that expansion (10) does not contain any disconnected terms. (5) The present model encompasses perturbative approaches in so far as the perturbative series for the reduced Green operators [$g_j^{(k)}$ in (17)] can be applied when necessary.

One of the simplest applications of Eq. (12) to condensed matter is the description of the propagation of two correlated hot electrons at surfaces. According to approximation (17), the total Green operator of two electrons moving in the surface crystal field is a product of three Green operators: the Green operators g_1 and g_2 of each of the individual electrons in absence of the inter-electronic coupling and the Green operator g_{12} of the electron pair in absence of the crystal. Expressions for g_1 and g_2 can be obtained from standard single particle band structure methods [2]. To evaluate g_{12} we need an expression for the electron–electron interaction in extended systems. This can be derived from the *GW* [6] method within the random phase approximation. A simplified version of this scenario has been implemented to study the excitation spectrum of an electron pair in a ferromagnetic surface [18]. When compared with experiments, the results are very promising and strongly indicate the validity of approximation (17) for this specific case.

References

- [1] K. Ohno, K. Esfarjani, Y. Kawazoe, Computational Material Science, Springer, Berlin, 1999.
- [2] I. Turek, V. Drchal, J. Kudrnovský, M. Šob, P. Weinberger, Electronic Structure of Disordered Alloys, Surfaces, and Interfaces, Kluwer Academic, Boston, 1997.
- [3] P. Fulde, Electron Correlation in Molecules and Solids, Springer Series in Solid-State Sciences, Vol. 100, Springer, Berlin, 1991.
- [4] R.M. Dreizler, E.K.U. Gross, Density Functional Theory, Springer, Berlin, 1990.
- [5] O. Schwartzkopf, B. Krässig, J. Elmiger, V. Schmidt, Phys. Rev. Lett. 70 (1993) 3008.
- [6] L. Hedin, J. Phys. C 11 (1999) R489.
- [7] R. Herrmann, S.N. Samarin, H. Schwabe, J. Kirschner, Phys. Rev. Lett. 81 (1998) 2148.
- [8] R. Wehlitz et al., Phys. Rev. Lett. 81 (1998) 1813.

- [9] I. Taouil, A. Lahmam-Bennani, A. Duguet, L. Avaldi, *Phys. Rev. Lett.* 81 (1998) 4600.
- [10] A. Dorn et al., *Phys. Rev. Lett.* 82 (1999) 2496.
- [11] M. Unverzagt et al., *Phys. Rev. Lett.* 76 (1996) 1043.
- [12] B. El-Marji, J.P. Doering, J.H. Moore, M.A. Coplan, *Phys. Rev. Lett.* 83 (1999) 1574.
- [13] R. Moshhammer et al., *Phys. Rev. Lett.* 84 (2000) 447.
- [14] For Coulomb potentials Eqs. (4), (12) can be used. However, when deriving state vectors or transition amplitudes an appropriate renormalization is required, such as the one suggested in J. Macek, *Phys. Rev. A* 37 (1988) 2365.
- [15] J.S. Briggs, *Phys. Rev. A* 41 (1990) 539.
- [16] B.A. Lippmann, *Phys. Rev.* 102 (1956) 264.
- [17] L.D. Faddeev, *Sov. Phys. JETP* 12 (1961) 1014.
- [18] J. Berakdar, *Phys. Rev. Lett.* 83 (1999) 5150.