Application of the Green Function Method for Calculating the Spatial Distribution of Electrons in the Finite System.

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Abstract. The paper presents a numerical implementation of the Green's function method for calculating the spatial distribution of the macroscopic number of free electrons in a finite system. The obtained results are compared with the results obtained by direct summation of the wave functions. The quantitative coincidence is demonstrated.

1. Introduction

In [1], [2], using several methodological approaches (an analytical method - the method of quasiclassical Green's functions, direct numerical summation of exact solutions for electronic wave functions), the spatial distribution of free electrons in the ground state in a finite spherical well was obtained. It was shown that the spatial distribution of electrons has a large spatial scale, which is of the order of the size of the system and is much larger than another spatial scale - the Fermi length of an electron. It is interesting to check the accuracy of the numerical technique used in [1], [2]. For this purpose, we present another numerical method for calculating the electron concentration based on the Green's function method. The obtained results are in a good quantitative agreement with the results obtained in [1], [2].

2. Construction of a Green function in the terms of two linearly independent solutions

A Green function of the Schrodinger equation is defined as a solution to the non-uniform equation

$$\left[ \frac{\hbar^2}{2m} \nabla^2 + V(r) - E \right] G(r, r') = \delta^{(3)}(r - r'). \quad (1)$$

This solution should satisfy boundary conditions specified by the quantum-mechanical problem considered. In the case of the spherically-symmetric potential $V(r)$ it is convenient to represent the Green function in the form of the partial-wave expansion [3]

$$G(r, r', E) = \frac{2m}{\hbar^2} \sum_{l=0}^{\infty} \frac{g_l(r, r')}{r \cdot r'} Y_{lm}^*(n_r) Y_{lm}(n_{r'}). \quad (2)$$

The common multiplier in Eq. (2) is chosen for convenience. Substituting this expansion into Eq. (1), we arrive to the following equation

$$\left[ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - v(r) + k^2 \right] g_l(r, r', k) = \delta(r - r'), \quad v(r) = \frac{2mV(r)}{\hbar^2}, \quad k^2 = \frac{2mE}{\hbar^2}, \quad (3)$$

for the partial Green functions $g_l(r, r', k)$. This is the non-uniform radial Schrodinger equation. The values $k$ and $E$ are connected by Eq. (3). The whole set of $g_l(r, r', k)$ is equivalent to the full function $G(r, r', E)$. Usually some restrictions for the orbital angular momentums arise in the most cases of
quantum-mechanical problems. Thus, it turns out that a finite set of terms is actually involved in summation in expansion (2).

The model potential (1) in the form of infinitely deep spherical well is adopted in the present study. The requirement of boundedness of a solution to Eq. (1) leads to the zero Dirichlet boundary condition at the origin for a solution to radial equation (3). The next boundary condition has the similar form and is imposed at the wall of the well.

The desired radial Green function \( g_j(r,r',k) \) can be expressed in terms of the two linearly - independent solutions \( \varphi_{1,2}(r) \) to the homogeneous equation (3). These solutions should satisfy the boundary conditions (4) and (5) respectively

\[
\varphi_1(0) = 0, \quad (4)
\]
\[
\varphi_2(R_0) = 0. \quad (5)
\]

Solutions \( \varphi_{1,2}(r) \) can be expressed by means of the already mentioned Riccati-Bessel functions

\[
\varphi_1(r) = kr \cdot j_l(kr), \quad (6)
\]
\[
\varphi_2(r) = \alpha \cdot kr \cdot j_l(kr) + \beta \cdot kr \cdot y_l(kr). \quad (7)
\]

The first solution \( \varphi_1(r) \) satisfies obviously condition (4). As concerning the second one \( \varphi_2(r) \) condition (5) implies

\[
\frac{\alpha}{\beta} = -\frac{y_l(kR_0)}{j_l(kR_0)}. \quad (8)
\]

The partial green function \( g_j(r,r',k) \) can be represented [3] in the following form

\[
g_j(r,r',k) = \frac{\varphi_1(r) \varphi_2(r)}{W_j[\varphi_1; \varphi_2]}, \quad (9)
\]

where \( r = \min(r, r'), R = \max(r, r') \), and \( W_j[\varphi_1; \varphi_2] - \) is Wronskian of the solutions \( \varphi_{1,2}(r) \)

\[
W_j[\varphi_1; \varphi_2] = \varphi_1(r) \frac{d\varphi_2(r)}{dr} - \varphi_2(r) \frac{d\varphi_1(r)}{dr} = k \beta. \quad (10)
\]

Eqs. (6)-(10) allow us to obtain the explicit expression for \( g_j(r,r',k) \)

\[
g_j(r,r',k) = \frac{1}{k} \left[ \frac{y_l(kR_0)}{j_l(kR_0)} \cdot (kr) \cdot j_l(\cdot kr) \cdot j_l(\cdot kr') \cdot j_l(\cdot kr') \cdot y_l(\cdot kr') \right]. \quad (11)
\]

This expression is applied here for numerical calculations.

3. Spatial density distribution: expression involving Green function

Let us consider the following model. Fermions occupy all the states below the Fermi energy \( E_F \) in the single-particle scheme. The density distribution can be rather simply related with the Green function. The most simple case is the problem with pure discrete spectrum. As it is clear from the Green’s function spectral decomposition

\[
G(r,r',E) = \frac{\sum_j u_j(r)u_j(r')}{E - E_j}, \quad (12)
\]

the spatial density is connected with an integral of function \( G(r,r',E) \) in the complex \( E \)-plane over a closed contour, that encloses all the poles related to the occupied states. In accordance with Cauchy’s integral formula this integral is equal to

\[
-2\pi \int_{E_j < E_F} \frac{u_j(r)}{E - E_j} \right|^2. \quad (13)
\]
Here the index \( j \) includes the whole set of quantum numbers indexing the state \((l,n)\). The numerical calculations can be based on the above mentioned contour integration.

It is worth to mention the following methodical aspect. Representation (2), (9) also allows to establish rather simply the similar conclusion. The eigenfunctions satisfy both the boundary conditions (4), (5). It means the coincidence of the solutions \( \varphi_1(r) \) and \( \varphi_2(r) \), and consequently the zeroing of the Wronskian in the denominator in Eq. (9). This corresponds to the pole of \( g_l(r,r',k) \). Let us examine more precisely the behavior of the Green function in the vicinity of the pole. In the following study we make use of the partial Green function explicit expression which has rather simple form (11) in the case considered. Heaving in mind the aim to calculate the contour integral, it is sufficient to pay attention to the pole term

\[
g_{ij}^{\text{pol}}(r,r',k) = -\frac{1}{k} \frac{j_i(kR_0)}{j_i(kR_0)} \left( kr \right) j_i(kr) \cdot \left( kr' \right) j_i(kr')
\]  

(14)

which contributes to the integral only. The other term has no singularities in every finite domain of the complex plane and does not contribute to the contour integral. The poles in (14) are related to the zeros \( z_{n,j} \) of the spherical Bessel function \( j_i(z) \). The approximate expression

\[
j_i(z) \approx j_i'(z_{n,j}) \cdot (z - z_{n,j}),
\]  

(15)

in the vicinity of a zero \( z_{n,j} \), follows from the Taylor series, retaining the major term. Eq. (15) allows one to obtain approximate simplified form of (8)

\[
\frac{\alpha}{\beta} \approx z - \frac{j_i\left(k_{n,l}R_0\right)}{j_i'(k_{n,l}R_0) \cdot (kR_0 - k_{n,l}R_0)}, \quad k_{n,l}R_0 \equiv z_{n,j}.
\]  

(16)

For our purposes Eq. (16) should be transformed in the following manner. Foremost it is desirable to express the numerator in Eq. (16) via the derivative \( j_i'(k_{n,l}R) \) with the help of the explicit Wronskian value

\[
W_\zeta[j_i(z); j_i'(z)] = j_i(z)j_i'(z) - j_i'(z)j_i(z) = \frac{1}{z^2}
\]  

(17)

and taking into account that \( z_{n,j} \) is a zero of the function \( j_i(z) \). The squared derivative \( \left[j_i'(z_{n,j})\right]^2 \) which arises in the denominator, should be replaced accordingly to the expression

\[
2\left[\left[x \cdot j_i(z_{n,j})\right]^2\right] dx = \left[j_i'(z_{n,j})\right]^2.
\]  

(18)

Relation (18) is a special case of the more common integral

\[
\int_0^x \zeta J_\nu^2(\lambda \zeta) d\zeta = \frac{2^2}{2} \left\{ \left[J_\nu'(\lambda x)\right]^2 + \left[1 - \frac{\nu^2}{(\lambda x)^2}\right]\left[J_\nu(\lambda x)\right]^2 \right\}
\]  

(19)

of the Lommel’s type. As a result of these transformations we arrive to the approximation for the term \( g_{ij}^{\text{pol}}(r,r',k) \) in the vicinity of a pole

\[
g_{ij}^{\text{pol}}(r,r',k) \approx \frac{\left(k_{n,l}r\right)j_i\left(k_{n,l}r\right) \cdot \left(k_{n,l}r'\right)j_i\left(k_{n,l}r'\right)}{\int_0^1 \left(\left(k_{n,l}\alpha\right)j_i\left(k_{n,l}\alpha\right)\right)^2 d\alpha} \cdot \frac{1}{2k(k-k_{n,j})}.
\]  

(20)

The first multiplier in Eq. (20) represents the product of the normalized radial eigenfunctions. The denominator of the second one can be transformed as follows

\[
2k(k-k_{n,j}) \approx (k + k_{n,j})(k - k_{n,j}) = k^2 - k_{n,j}^2
\]

for \( k \) in the vicinity of \( k_{n,j} \). As expected, the pole parameters (the location and the residue) are the same as for the respective term in spectral decomposition (12).
The consideration of the concrete model problem presented above allows one to trace clearly the interrelation of the two types of Green function representations—spectral decomposition and by means of two linearly independent solutions. The aim of the presented consideration includes not only the methodical aspect but also comprise practical recipe for calculation of the spatial density. We shall discuss some aspects, connected with numerical procedures realized here. Let us pay attention to the fact that it is sufficient to account for the pole term (14) of the Green function only. Contour integration in the complex $E$-plane can be transformed to contour integration in the complex $k$-plane, which occurs more convenient for numerical calculations.

Fig. 1 represents one of the possible choices of the closed contour for integration. This contour is chosen in the form of rectangle ABCD and encloses the set of poles located to the left from $k_F$. It is sufficient to provide calculation of the imaginary part of the integral only. Contributions of the segments AB and CD into the integral can be neglected if their lengths are sufficiently small. The further simplification can be attained taking into account the fact that the Green function values for the conjugated values of $k$ are also conjugated. Thus one can reduce the calculation procedure to integration of the imaginary part of the integrand over the segment DA only, provided that this segment located rather close to the real axis. This observation reduces amount of calculations significantly. The next point of the numerical procedures is calculations of the Bessel functions, having in mind a small imaginary admixture in argument. Calculation of the function $y_l(z)$ does not cause difficulties usually. Recurrence relations turn out effective and reveal stability in the upward direction. Thus all necessary values $y_l(z)$ can be determined recurrently, starting from the initial ones, calculated for $l=0$ and 1 with the aid of the explicit expressions [4].

As concerning $j_l(z)$ values, recurrence procedure should be organized in the downward direction. Asymptotic values at extremely large index $l$ can serve as starting values. Continued fractions are also efficient together with recurrence relations. The Bessel function values $j_l(z)$ calculated recurrently can be corrected comparing the value $j_0(z)$ and the one obtained from explicit expression. On the whole, these techniques allow one to calculate rather effectively Green function for the problem considered. Details of computational algorithms for Bessel functions are presented in Refs. [5].

![Fig. 1. Contour of integration.](image-url)
Using the described technique, the electron concentration was calculated for two systems. These results are shown in Fig. 2 (blue curves). We also show similar calculations obtained by direct summation of wave functions (red curves). The quantitative coincidence is demonstrated. It indicates a good accuracy of the developed numerical methods for calculating the electron concentration.

Fig. 2 Spatial electron concentrations. Blue curves - Green function method, red curves - direct summation of wave functions.

4. Conclusion

The paper presents a computational method for calculating the spatial distribution of free electrons in the ground state in a spherical indefinite well. The method is based on the numerical calculation of the exact Green’s function of the system, which is used to determine the electron concentration. The results obtained by the developed numerical technique are in a good numerical agreement with the results obtained earlier by direct summation of the wave functions. This result indicates a good accuracy of the developed numerical methods for calculating the electron concentration.

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