Quantum-Mechanical Analysis of Single Particle Level Density*

I. Ţetcu†

Institute for Nuclear Physics and Engineering "Horia Hulubei",
P.O. Box MG-6, 76900 Bucharest, Romania

A quantum-mechanical calculation of the single-particle level (s.p.l.) density $g(\varepsilon)$ is carried on by using the connection with the single-particle Green’s function. The relation between the imaginary part of Green’s function and single-particle wave functions is used separately for the discrete and continuous states. Within the bound-states region the imaginary part of the Green’s function is calculated by using the wronskian theorem. The Green’s function corresponding to the continuum is written by using the regular and Jost solutions of the radial Schrödinger equation. The smooth part of the rapidly fluctuating s.p.l. density is calculated by means of the Strutinski procedure. The continuum component of the s.p.l. density has rather close values within either exact quantum-mechanical calculations with the Woods-Saxon (WS) potential, or Thomas-Fermi approximation with WS as well as finite-square potential wells, provided that the free-gas contribution is subtracted. A similar trend is obtained by means of the simple FGM formula for the s.p.l. density if the continuum effect is taken into account.

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I. INTRODUCTION

The nuclear level density has a central role in the statistical analysis of nuclear reactions. Information concerning nuclear densities can be obtained from experiments by means of the analysis of neutron and charged particles resonances, inelastic scattering, and particle evaporation spectra, so that the theoretical calculation of this quantity is quite useful for validation of nuclear models. Many approaches (e.g. [1–3] and references therein) have been developed to calculate the single-particle level (s.p.l.) density on which is based the nuclear level density calculation, its establishment being yet considered a difficult task. A constant s.p.l. density $g \sim A/14$ MeV$^{-1}$ was used in various statistical model descriptions of the nuclear reactions. An increased criticism has been expressed on this constant value which is inconsistent with the number of $A$ nucleons in the nucleus and the usual Fermi energy $F = 38$ MeV.

The semiclassical approximations could be the starting point of a basic analysis of the s.p.l. density, including the energy dependence. First, the Thomas-Fermi approximation proves adequate for a special class of potential wells [1] which describe the nuclear mean field (Woods-Saxon, harmonic oscillator, trapezoidal potential well). However, for potentials like square-well and infinite square potential, the results deviate significantly from the quantum-mechanical calculation. Enhanced approximations add the lowest terms in $\hbar$ as corrections to the Thomas-Fermi results [2,3].

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†stetcu@roifa.ifa.ro
An exact quantum-mechanical calculation was provided by Shlomo [1] by using a Green’s function approach. A particular case is the s.p.l. density for a finite potential well. Since it is including the free-gas states, one can calculate and subtract this component by using the Green’s function associated with the respective single-particle Hamiltonian. Shlomo found by means of both semiclassical and quantum methods that, for a realistic finite depth potential well, the s.p.l. density decreases with energy in the continuum region (the continuum effect).

The paper is organised as follows. Section II is an introduction of the general theoretical aspects concerning the s.p.l. density, namely the definition, its relation with the Green’s function, the Strutinski smoothing procedure, and semiclassical methods usually involved. Section III gives a general description of the single particle Green’s function theory and a method for the calculation of its imaginary part. The model parameters for the mean field potential and numerical results are discussed in section IV. Finally, the conclusions are drawn in section V.

II. BASIC FORMALISM FOR SINGLE-PARTICLE LEVEL DENSITY

A. The quantum-mechanical single-particle level density

A brief presentation of the s.p.l. density definition, Green’s function and relation between them are given in this section. The s.p.l. density is defined as [1]

\[ g(\varepsilon) = \text{Tr}(\delta(\varepsilon - \hat{H})) , \]

where \( \hat{H} \) is the corresponding single-particle Hamiltonian (mean field)

\[ \hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(r) . \]

The eventual bound states of the Hamiltonian given by Eq. (2) can be obtained from the time independent Schrödinger equation

\[ \hat{H}|n\alpha\rangle = \varepsilon_n|n\alpha\rangle , \]

\( \alpha \) being the degeneracy given by other quantum numbers. It is supposed that the normalisation for the eigenvectors corresponding to bound states is

\[ \langle n'\alpha'|n\alpha\rangle = \delta_{nn'}\delta_{\alpha\alpha'} , \]

so that the s.p.l. density following Eq. (1) is

\[ g_B(\varepsilon) = \sum_{n\alpha} \delta(\varepsilon - \varepsilon_n) . \]

In the case of a finite potential well which has bound as well as continuous states the s.p.l. density can be considered for the two regions of the spectrum

\[ g(\varepsilon) = g_B(\varepsilon) + g_C(\varepsilon) , \]

where \( g_B(\varepsilon) \) and \( g_C(\varepsilon) \) are the contributions given by the bound and continuous states respectively. The continuum contribution are determined from the scattering phase shifts \( \delta_{ij}(\varepsilon) \) by [1,4]

\[ g_C(\varepsilon) = \frac{1}{\pi} \sum_{ij} (2j + 1) \frac{d\delta_{ij}(\varepsilon)}{d\varepsilon} . \]
It can be determined also from Eq. (1) but the eigenvectors corresponding to the continuum states can not be normalised similarly to the bound states case. The relation (3) becoming

\[ \langle \varepsilon' \alpha' | \varepsilon \alpha \rangle = \delta(\varepsilon - \varepsilon')\delta(\alpha - \alpha') , \]  

it results

\[ g_C(\varepsilon) = \sum_{\alpha'} \int d\varepsilon' \delta(\varepsilon - \varepsilon') \langle \varepsilon' \alpha' | \varepsilon' \alpha' \rangle , \]  

where the sum after \( \alpha' \) can be an integral if this parameter is continuous. For the moment we will assume that the states are not degenerate so that the s.p.l. density in the whole energy range has the form

\[ g(\varepsilon) = \sum_n \delta(\varepsilon - \varepsilon_n) + \int d\varepsilon' \delta(\varepsilon - \varepsilon') \langle \varepsilon' | \varepsilon' \rangle . \]  

An important quantity is the number of states \( N(\varepsilon) \) with energy below \( \varepsilon \), which will be used latter for illustration of the continuum effect,

\[ N(\varepsilon) = \int_{-\infty}^{\varepsilon} d\varepsilon' g(\varepsilon') . \]  

By means of the condition

\[ A = \int_{-\infty}^{\varepsilon_F} d\varepsilon g(\varepsilon) , \]  

Eq. (8) can be also used for determination of the Fermi energy \( \varepsilon_F \) which is a significant quantity for the description of the nucleus ground state or nuclear reactions analysis.

**B. The Green’s function approach**

The single-particle Green’s function \( G(\mathbf{r}, \mathbf{r}'; \varepsilon) \) corresponding to the Hamiltonian (2) is defined by the equation \[ \[ (\varepsilon - \hat{H})G(\mathbf{r}, \mathbf{r}'; \varepsilon) = \delta(\mathbf{r} - \mathbf{r}') . \]  

A first assumption has considered the nucleus in a large volume \( \Omega \) \( (i.e. \) within an infinite potential well), the continuum being discretized. In this case, the spectral representation of the Green’s function

\[ G(\mathbf{r}, \mathbf{r}'; \varepsilon) = \sum_n \frac{\langle \mathbf{r} | n \rangle \langle n | \mathbf{r}' \rangle}{\varepsilon - \varepsilon_n} \]  

can be used to obtain

\[ \lim_{\alpha \to 0^+} \frac{1}{2\pi i} \int d\mathbf{r} \lim_{\mathbf{r}' \to \mathbf{r}} (G(\mathbf{r}, \mathbf{r}'; \varepsilon + i\alpha) - G(\mathbf{r}, \mathbf{r}'; \varepsilon - i\alpha)) \]

\[ = \frac{1}{2\pi i} \lim_{\alpha \to 0^+} \sum_n \left( \frac{1}{\varepsilon - \varepsilon_n + i\alpha} - \frac{1}{\varepsilon - \varepsilon_n - i\alpha} \right) = - \sum_n \delta(\varepsilon - \varepsilon_n) , \]  

where it has been used the well-known relation \[ 3 \]
\[
\lim_{\alpha \to 0^+} \frac{1}{x-a \pm i\alpha} = \frac{P}{x-a} \mp i\pi \delta(x-a).
\]

By comparison of the Eqs. (4) and (11) it results the following relation between the s.p.l. density and Green's function (see also [6])

\[
g(\varepsilon) = -\frac{1}{\pi} \lim_{\alpha \to 0^+} \int dr \lim_{r \to r'} \Im(G(r, r'; \varepsilon + i\alpha)). \tag{12}
\]

The demonstration can be generalised at this point for the both sides of the spectrum. Without consideration of the nucleus in a finite volume Eq. (10) becomes

\[
G(r, r'; \varepsilon) = \sum_n \langle r|n\rangle\langle n|r'\rangle \varepsilon - \varepsilon_n + \int d\varepsilon' \langle r|\varepsilon'\rangle\langle \varepsilon'|r'\rangle \frac{\varepsilon - \varepsilon'}{\varepsilon - \varepsilon'} \tag{13}
\]

while an integral corresponding to the continuum energy range is added similarly to the sum in Eq. (11). Next, within this additional term it can be used the relation

\[
\int dr \langle r|\varepsilon'\rangle\langle \varepsilon'|r\rangle = \langle \varepsilon'|\varepsilon'\rangle,
\]

so that the respective continuum contribution becomes just the second term in Eq. (7). Therefore, Eq. (12) is proved worthy not only for the bound states but in the general case.

Next, the dependence of the s.p.l. density by \(\varepsilon\) and \(r\) can be expressed as

\[
g(\varepsilon, r) = -\frac{1}{\pi} \lim_{\alpha \to 0^+} \Im G(r, r'; \varepsilon + i\alpha) \bigg|_{r \to r'} \tag{14}
\]

It is reduced to the dependence by \(\varepsilon\) and \(r\) in the common case of a central potential.

The s.p.l. density for the free particles without spin, i.e. for \(V(r) = 0\) in Eq. (2) can be also obtained for Eqs. (12) and (14). The single particle Green's function in this case is

\[
G_0^{(+)}(r, r'; \varepsilon) = \lim_{\alpha \to 0^+} G_0(r, r', \varepsilon + i\alpha) = -\frac{2m \exp(iR/\hbar)}{\hbar^2 4\pi |R|}, \tag{15}
\]

where \(R = r - r'\) and \(k = \sqrt{2m\varepsilon/\hbar^2}\).

Introducing Eq. (15) in Eq. (14)

\[
g_0(\varepsilon, r) = -\frac{1}{\pi} \lim_{R \to 0} \Im \left[ -\frac{2m \exp(iR/\hbar)}{\hbar^2 4\pi R} \right]
\]

\[
= \frac{2m}{4\pi^2 \hbar^2} \lim_{R \to 0} \left[ \sin(kR) \right] R, \tag{16}
\]

it results the expected characteristic of \(g_0(\varepsilon, r)\) to be a function of only \(\varepsilon\), for the case of free particles

\[
g_0(\varepsilon, r) = \frac{1}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \sqrt{\varepsilon}. \tag{17}
\]

Furthermore, by using Eq. (17) in Eq. (12) one obtains the well-known formula of the s.p.l. density for free particles without spin restricted to a finite volume \(\Omega\) [1].
\[ g_0(\varepsilon) = \frac{\Omega}{4\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \sqrt{\varepsilon}. \] (18)

We have to pay attention at the numerical calculation of the limit \( \alpha \to 0_+ \) in Eq. (12). The s.p.l. density could be calculated by smearing of the Green’s function with a Lorentz function of small width \( \gamma \). By using the relation

\[ \lim_{\alpha \to 0_+} \gamma \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\varepsilon'}{(\varepsilon' - \varepsilon)^2 + \gamma^2} G(\mathbf{r}, \mathbf{r}'; \varepsilon' + i\alpha) = G(\mathbf{r}, \mathbf{r}'; \varepsilon + i\gamma), \] (19)

the smeared level density \( g_\gamma(\varepsilon) \) can be obtained from Eq. (12) while \( \alpha \) is replaced by a finite but small value of \( \gamma \). This parameter should have a value much smaller than \( \hbar\omega \), the spacing between major shells. The method is used in several studies [1,3,7] and has the advantage that the knowledge of the spectrum of \( \hat{H} \) is not any more necessary.

Alternatively, an analytical calculation of the single-particle Green’s function is adopted in the present work, in order to obtain an exact form of the s.p.l. density within the continuum region too. Because of the differences between the regular and irregular solutions of the radial Schrödinger equation for the two regions of the spectrum, the respective limits \( \alpha \to 0_+ \) in Eq. (14) have to be calculated separately as it is shown in section III.

C. The smoothing procedure

The level density \( g(\varepsilon) \) varies rapidly with energy, due to the shell effects. However, besides its rapidly fluctuating part, \( g(\varepsilon) \) contains a smooth part describing the average behaviour of the level distribution [4,8]

\[ g(\varepsilon) = g_s(\varepsilon) + \delta g(\varepsilon). \]

For the discrete states, the smooth part of the level density can be obtained from Eq. (12) by smearing out each \( \delta \) function to a Gaussian of width \( \Gamma \) [4]

\[ \delta(\varepsilon - \varepsilon_n) \to \frac{1}{\Gamma \sqrt{\pi}} \exp \left[ - \left( \frac{\varepsilon - \varepsilon_n}{\Gamma} \right)^2 \right], \]

where \( \Gamma \) should be at least of the order of the shell spacing. Although such a Gaussian preserves the normalisation of a \( \delta \)-function, curvature corrections have to be introduced in such a way that not only \( g_s(\varepsilon) \) but also its first \( 2M \) derivatives are reproduced correctly [4,8]. The unitary treatment of the bound and continuous states is realized by means of an average of the s.p.l. density (Strutinski’s procedure) [4]

\[ g_s(\varepsilon) = \int_{-\infty}^{\infty} d\varepsilon' F(\varepsilon - \varepsilon') g(\varepsilon'), \] (20)

where

\[ F(x) = \frac{1}{\Gamma \sqrt{\pi}} e^{-\left( \frac{x}{\Gamma} \right)^2} L^2_M(x^2/\Gamma^2), \]

and \( L^2_M \) is the associated Laguerre polynomial [9]. The smoothing parameter \( \Gamma \) has to be chosen [4,8] greater than \( \hbar\omega \).
D. Subtracting the free gas contribution

The background level density due to the free Fermi gas (which goes like $\sqrt{\varepsilon}$) exists whether or not the potential well is finite [4], the former case yielding the quantum fluctuation of the density. A subtracting procedure was introduced by Shlomo [1–3], the states corresponding to the free Hamiltonian $\hat{H} = \hat{P} / 2m$ being taken away for $\varepsilon > 0$

$$g(\varepsilon) = \int d\mathbf{r} \left( g(\varepsilon, \mathbf{r}) - g_0(\varepsilon, \mathbf{r}) \right).$$  \hspace{1cm} (21)

Therefore, the s.p.l. density decreases with energy in the continuum region (the so called continuum effect).

A particular problem occurs for protons. The corresponding free gas contribution has to be considered with the Coulomb interaction included. The smoothing procedure (20) will be involved following the subtraction of the free gas contribution.

E. Semiclassical calculation of $g_s(\varepsilon)$

The semiclassical approximations for calculation of the s.p.l. density are commonly used [1,2,10]. The $\hbar$-expansion (Wigner-Kirkwood) of the single-particle partition function is used in this respect [10], performing the so-called Wigner transform. The terms with odd power of $\hbar$ vanish for the smooth single-particle potentials. Therefore, the Thomas-Fermi (TF) approximation ($\hbar^0$ term) and the semiclassical (SC) approximation (TF+$\hbar^2$ correction) are generally considered. The numerical calculations in this work have been carried out for the TF-method only. The results of the TF approximation by taking into account the spin degeneracy and neglecting the spin-orbit interactions are given in several papers [1,2,10]

$$g_{TF}(\varepsilon) = \frac{1}{2\pi} \left( \frac{2m^2}{\hbar} \right)^{3/2} \int d\mathbf{r} \left( \varepsilon - V(\mathbf{r}) \right)^{1/2} \Theta(\varepsilon - V(\mathbf{r})).$$  \hspace{1cm} (22)

For the finite well potentials we have to subtract [1,2] the contribution of free Fermi gas when $\varepsilon > 0$, which is given by Eq. (17).

III. SINGLE-PARTICLE GREEN’S FUNCTION CALCULATION

In this section a partial wave analysis for Green’s function is presented for particles with spin $\frac{1}{2}$. A brief review of some elements which are necessary for such description of particles is given firstly.

Let $\chi_{\nu}^s$ and $C(lsj, m\nu M)$ be the normalised eigenvectors of the spin, and respectively the Clebsch-Gordan coefficients. By using spherical harmonics $Y_{lm}(\hat{r})$ there are defined the functions [5]

$$Y_{jls}^M(\hat{r}) = \sum_{m\nu} C(lsj, m\nu M)Y_{lm}^m(\hat{r})\chi_{\nu}^s.$$  \hspace{1cm} (23)

They are eigenfunctions of the total angular-momentum operator, its $z$ component (with respect to a given $z$ axis), the orbital angle-momentum operator, and the spin operator.

Following the expansion of the Green’s function [3]
the partial-wave Green’s function \( G_{ij}^{(\pm)}(r, r'; \varepsilon) \) satisfies the equation

\[
\left( -\frac{\partial^2}{\partial r^2} + \frac{l(l + 1)}{r^2} - k^2 + \frac{2m}{\hbar^2} V_{lj}(r) \right) G_{ij}^{(\pm)}(r, r'; \varepsilon) = -\delta(r - r')
\]

with the boundary conditions specifying that it is zero at \( r = 0, \) for fixed \( r' \) and at \( r \to \infty \) it contains outgoing (for \( G^{(+)} \)) or incoming waves (for \( G^{(-)} \). The solution of Eq. (25) can be expressed by using the regular \( u_{lj}(r) \) and irregular solutions \( v_{lj}^{(\pm)}(r) \) of the radial equation,

\[
G_{ij}^{(\pm)}(r, r'; \varepsilon) = \frac{u_{lj}(r_<) v_{lj}^{(\pm)}(r_>)}{W_{lj}},
\]

where \( W_{lj} \) is the wronskian of the two solutions, and \( r_< \) and \( r_> \) are the lesser and the greater of \( r \) and \( r' \), respectively. The regular solutions are defined for \( r \to 0 \) so that it is satisfied the boundary condition

\[
u_{lj}(r = 0) = 0.
\]

Because of the hermiticity of the Hamiltonian, the regular solution can be chosen real. The irregular solutions are defined for \( r \to \infty \) by

\[
v_{lj}^{(\pm)}(r) \big|_{r \to \infty} \sim \begin{cases} e^{-\kappa r} & \text{if } \varepsilon < 0 \\ e^{\pm ikr} & \text{if } \varepsilon > 0, \end{cases}
\]

where \( \kappa = \sqrt{-2m\varepsilon/\hbar^2} \).

**A. Bound-states region (\( \varepsilon < 0 \))**

The imaginary part of \( G(r, r; \varepsilon + i\alpha) \) is obtained following the calculation of the limit \( \alpha \to 0_+ \). Moreover, we have to pay attention to the both possibilities for \( \varepsilon \) to be or not an eigenvalue. In the first case, since the regular and irregular solutions can be chosen real and are linearly independent, the limit in Eq. (12) is easy to perform and the imaginary part of Green’s function becomes zero.

In the second case the regular \( u(r) \) and irregular solution \( v(r) \) are linearly dependent, so that it results

\[
u_{lj}(r) = C_{lj} v_{lj}(r),
\]

where the coefficient \( C_{lj} \) can be obtained from the boundary conditions.

Let \( \varepsilon_0 \) be an eigenvalue, and \( K_0 \) a complex number given by

\[
K_0 = \sqrt{\frac{2m(\varepsilon_0 + i\alpha)}{\hbar^2}} = i\kappa_0 - \alpha',
\]

where \( \alpha' \to 0_+ \). The wronskian can be expanded around \( \alpha' \)
\[ W_0(K_0) = -\frac{\partial W_0}{\partial K_0} \bigg|_{K_0=i\kappa_0} \alpha' + O(\alpha'^2), \]  

(30)

while the use of the wronskian theorem leads to [3][11]

\[ \frac{\partial W_0}{\partial K_0} = -\frac{K_0}{C_0} \int_0^\infty dr u^2_{ij}(r). \]  

(31)

The imaginary part of the Green’s function can be calculated now by using Eqs. (26) and (31). The result is a sum of $\delta$-functions

\[ \text{Im} \,(G(r, r; \varepsilon)) = \sum_n D_n u^2_n(r) \delta(\varepsilon - \varepsilon_n). \]  

(32)

Finally, by introducing Eq. (32) in Eq. (12) and comparing with Eq. (4), the coefficients $D_n$ can be obtained and the s.p.l. density at negative energies becomes

\[ g(\varepsilon, r) = \sum_n u^2_n(r) \delta(\varepsilon - \varepsilon_n), \]  

(33)

where it has been assumed the following normalisation condition for the regular solutions

\[ \int_0^\infty dr u^2_n(r) = 1. \]

The solutions of the radial Schrödinger equation considered in this frame

\[ \frac{\hbar^2}{2m} \frac{d^2 u_n(r)}{dr^2} + \left[ \varepsilon_n - V(r) - \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right] u_n(r) = 0, \]  

(34)

have been obtained for $V(r)$ being the sum of the Woods-Saxon (WS) nuclear potential and the Coulomb potential in the case of protons. The former has the expression

\[ V^{WS}(r) = \frac{V_0}{1 + \exp[(r-R)/a_0]}, \]  

(35)

where $V_0 < 0$, $R$ and $a_0$ are the depth, the radius and the diffuseness parameters of the well, respectively (given within the following section), while the latter is

\[ V_c(r) = \begin{cases} \frac{Z e^2}{2 R_c} \left( 3 - \frac{r^2}{R_c^2} \right) & r < R_c \\ \frac{Z e^2}{r} & r > R_c, \end{cases} \]  

(36)

for a uniformly charged sphere of radius $R_c$. The boundary conditions satisfied by these solutions are

\[ u_n(0) = 0 \]

\[ u_n(r)|_{r\to\infty} \to 0. \]

The eigenvalues of the WS potential well, which can not be found analytically, have been obtained by using the Nilsson-orbits computer code developed by Hird [12]. A basis of harmonic oscillator eigenstates
\[ R_{nl}(r) = \left[ \frac{2\lambda^{3/2}n!}{\Gamma(n + l + \frac{3}{2})} \right]^{1/2} (\lambda r^2)^{l+\frac{1}{2}} (\lambda r^2) \exp \left( -\frac{\lambda r^2}{2} \right) \]

has been used, with the condition for the best convergence of the WS states in the harmonic potential given by the relation \[ \lambda = 0.15466 \sqrt{\frac{|V_0|}{R}}, \] (37)

between the size parameter and the parameters of the well, where the energies are in MeV and the lengths in fm. Illustrative results of the numerical integration of Eq. (34) by using this method are shown in Fig. 1.

![Graph showing Woods-Saxon nuclear potential shape and corresponding radial wave functions for neutrons.](image)

**FIG. 1.** (a) The Woods-Saxon nuclear potential shape for the global parameter set given, and (b) corresponding radial wave functions for neutrons.

### B. Continuum-energy region \((\varepsilon > 0)\)

The methods used in this work for evaluation of the s.p.l. density within the bound-states and continuum regions, respectively, are distinct. There are two linearly independent solutions for the radial Schrödinger equation, defined by various boundary conditions

\[ u_{lj}(r) \to \sin \left( kr - \frac{\varepsilon l}{2} + \delta_{lj} \right) \text{ when } r \to \infty, \] (38)

and

\[ \tilde{u}_{lj}(r) \to \cos \left( kr - \frac{\varepsilon l}{2} + \delta_{lj} \right) \text{ when } r \to \infty. \] (39)

Eq. (38) is providing the regular solution \( u_{lj}(r) \), while Eqs. (38) and (39) can be used to obtain the irregular solution (Jost solution) \( v_{lj}^{(\pm)}(r) \) satisfying the condition given by Eq. (28),
\[ v_{lj}^{(\pm)}(r) = \tilde{u}_{lj}(r) \pm iu_{lj}(r). \] (40)

The wronskian of the two solutions is \( r \)-independent (according to the wronskian theorem) with the result \( W_{lj} = -k \). Consequently, the imaginary part of Green’s function becomes

\[ \text{Im} \left( G_{lj}^{(+)}(r, r; \varepsilon) \right) = -\frac{u_{lj}^2(r)}{k}. \] (41)

Therefore, the \( r \)- and \( \varepsilon \)-dependent s.p.l. density for \( \varepsilon > 0 \) is

\[ g(\varepsilon, r) = \frac{2m}{\pi \hbar^2} k \sum_{lj} (2j + 1) u_{lj}^2(r), \] (42)

i.e. it is given only by the regular solution of the radial Schrödinger equation corresponding to the potential well.

The latest equations can be used for the calculation of the s.p.l. density for free particles too. The regular solution in this case is given by

\[ u_{lj}^0(r) = kr j_l(kr), \] (43)

where \( j_l(kr) \) is the spherical Bessel function, regular in origin, and \( g_0(\varepsilon, r) \) becomes

\[ g_0(\varepsilon, r) = \frac{2m}{\pi \hbar^2} kr^2 \sum_{lj} (2j + 1) j_l^2(kr). \] (44)

Since \( 2j + 1 = 2(2l + 1) \) in the general case of a single-particle potential which neglect the spin-orbit interaction, it results by using the relation \[ \sum_{l=0}^{\infty} (2l + 1) j_l^2(x) = 1, \]

that \( g_0(\varepsilon, r) \) is the same as given by Eq. (17) except the spin degeneracy is taking into account

\[ g_0(\varepsilon, r) = \frac{4m}{\pi \hbar^2} kr^2. \]

This result is an useful test for the correctness of the relation (42) which has been in this work the starting point for the numerical calculation of the s.p.l. density in the continuum region.

The numerical solutions of the Schrödinger equation have been obtained by using the Cowell method [13,14]. A modified version of the optical model code SCAT2 [14] has been used in this respect. The results of the numerical integration for neutrons is shown in Fig. 2.

The solutions are conveniently defined by the condition that they are given asymptotically, e.g. for neutrons, by

\[ u_{lj}(r) = \sin \left( kr - \frac{l\pi}{2} + \delta_{lj} \right) \quad \text{when} \ r \rightarrow \infty, \] (45)

where \( \delta_{lj} \) is the phase shift corresponding to the mean-field potential. In particular, the phase shift can be used in the calculation of the differential cross section [3,11] for the particles scattered on a finite-range potential (for the Coulomb potential can be also made). The s-wave phase shift for the WS potential well is shown as a function of energy in Fig. 2(b).
FIG. 2. The s-wave radial solution of the Schrödinger equation in continuum, for the Woods-Saxon potential (solid curve) as well as without it (dotted curve), and (b) the corresponding s-wave neutron phase shift, for the nucleus $^{93}$Nb.

IV. MODEL PARAMETERS AND RESULTS

The quantum-mechanical and TF calculations of the s.p.l. density for neutrons within the nucleus $^{56}$Fe have been carried out by using the following potential wells. The respective parameters were determined by looking for the available experimental data on nuclear radii and separation energies to be reproduced by the corresponding single-particle Hamiltonian $^1$.

A. Potential well parameters

(i) The harmonic-oscillator (HO) potential as sample of an infinite potential well, but with a smooth surface and applicable only for $A \leq 100$, is given by

$$V^{HO}(r) = \frac{1}{2}m\omega^2r^2,$$

(46)

where the parameterisation $^1$ $\bar{\hbar}\omega = 45\frac{A^{1/3}}{A^{1/3}} - 25\frac{A^{2/3}}{A^{2/3}}$ (MeV)

(47)

has been adopted. On the other hand, the usual size parameter of the potential $\lambda = m\omega/\hbar$ has been replaced according to Eq. (37) for the basis of HO eigenstates which is used for the expansion of the WS potential eigenstates, for a better convergence of the numerical method $^{12}$.

(ii) The infinite square-well (SQ) potential of the form

$$V^{SQ}(r) = \begin{cases} V_0, & r < R \\ \infty, & r > R \end{cases},$$

(48)

has been used with the depth and radius parameters
\[ V_0 = -46 + 33 \frac{N-Z}{A} t_3 \text{ (MeV)}, \]

\[ R = R_V = 1.12A^{1/3} + 1.6 \text{ fm}, \]

Actually, it is the basis for the Fermi-gas model (FGM) of the nucleus. The respective eigenvalues are provided by the boundary condition for the single-particle wave functions to vanish at the nuclear surface \((r = R)\) while the square-root energy dependence of the s.p.l. density is given by, e.g., the semiclassical Thomas-Fermi formula \((\text{TF})\).

(iii) The finite square (FSQ) potential of the form

\[
V_{FSQ}(r) = \begin{cases} V_0 & r < R \\ 0 & r > R \end{cases},
\]

has been used, with the depth \(V_0 = -47 + 33 \frac{N-Z}{A} t_3 \text{ (MeV)},\)

where \(t_3=1\) for a neutron and \(-1\) for a proton, while the radius has the same value as for the WS potential well.

(iv) The WS potential well parameters within Eq. (35) as given by Shlomo's global set are \(V_0 = -54 + 33 \frac{N-Z}{A} t_3 \text{ (MeV)}, R = \frac{R_V}{1 + (\pi a/R^{1/3})}, \quad R_V = 1.12A^{1/3} + 1.0 \text{ fm} \)

\[ a = 0.70 \text{ fm}, \]

where \(R\) is determined by iteration.

**B. Results and discussion**

The number of the bound single-neutron states with the energy less than \(\varepsilon\), i.e. \(N(\varepsilon)\) given by Eq. (8), is shown in Fig. 3(a) as a function of \(\varepsilon\) for the nucleus \(^{40}\text{Ca}\), by using the WS potential within the both QM and TF methods. It is found similarly to Shlomo \(\text{[1]}\) that, in the case of the WS smooth potential, the TF formula may be considered a good approximation of the quantum-mechanical results. Additionally, in Fig. 3(b) is shown the effect of the free-gas contribution subtracting, in the frame of the TF approximation.

The continuum effect on the s.p.l. density for neutrons is firstly shown within the TF method, in the case of the nucleus \(^{56}\text{Fe}\). The use of the infinite square-well provides the usual s.p.l. density of the Fermi-gas model. At the same time the respective finite well determines the continuum region of the spectrum where the consideration of the free-gas contribution by Eq. (21) is illustrated in Fig. 4(a). Next, the same effect in the TF approximation but using the realistic WS potential well is shown in Fig. 4(b). It could be noted that, in spite of the quite distinct energy dependences due to the SQ and WS potentials wells, the continuum components are rather similar following the proper consideration of the free-gas contribution.

The analysis of the continuum effect is completed by the quantum-mechanical calculation for the same neutron level density of the nucleus \(^{56}\text{Fe}\) in the Woods-Saxon potential well. The smooth
FIG. 3. The number of single-neutron states $N(\varepsilon)$ as a function of $\varepsilon$ for the nucleus $^{40}\text{Ca}$ and the Woods-Saxon potential, given by (a) the quantum-mechanical calculated single-particle energies (histogram), and the TF approximation (dotted curve), and (b) the latter method with (solid curve) and without (dotted curve) the free-gas contribution subtracted.

FIG. 4. The s.p.l. density for neutrons of the nucleus $^{56}\text{Fe}$ as a function of the single-particle energy, given by the TF approximation with (a) the infinite square-well (dashed curve), finite square potential well (solid curve), and (b) the Woods-Saxon potential (dashed curve), as well as by the smoothed quantum-mechanical calculation with the same WS potential well (solid curve). The dotted curve correspond to the QM calculation carried out without subtraction of the free-gas contribution.

level density obtained by using the smooth parameter $\Gamma = 1.2\hbar\omega$, where $\hbar\omega$ is given by Eq. (47), and the order of Laguerre polynomial $M=2$, is shown in Fig. 4(b) too. The comparison with the results of the TF approximation, which involves the same potential well, proves the suitability
FIG. 5. The same as Fig. 4, for the quantum-mechanical calculation with the WS potential (solid curve), TF approximation with the FSQ potential well (dashed curve), and the FGM formula with the Fermi energy values of $F=38$ MeV (dotted curve) and $F=20$ MeV (dash-dotted curve).

of the latter similarly to that previously by Shlomo [1].

Actually, it results that the continuum component of the s.p.l. density has rather close values within either exact QM calculations with the WS potential, or TF approximation with WS as well as FSQ potential wells, provided that the free-gas contribution is subtracted. Moreover, a similar trend is obtained by means of the simple FGM formula for the s.p.l. density (e.g., [15]), if the continuum effect is taken into account (Fig. 5). The level of agreement between this phenomenological formula and the QM calculation could be improved for lower values of the Fermi energy $F$ which is usually considered $\sim 38$ MeV [16]. It is thus even possible to reproduce the quantum-mechanical results by using the average Fermi energy $F \sim 20$ MeV which is determined by the nuclear-surface localization of the first nucleon-nucleon collision in preequilibrium reactions [17, 18].
FIG. 6. The smooth s.p.l. density for the nucleus $^{40}$Ca as a function of the single-particle energy, given by (a) quantum-mechanical (solid curve) and TF approximation (dashed curve), for neutrons, and (b) QM calculations for neutrons (dotted curve) as well as protons (dashed curve) and their sum (solid curve).

Finally, the smoothed results of the quantum-mechanical calculation for the s.p.l. density of neutrons as well as protons in the nucleus $^{40}$Ca are shown in Fig. 6(b). In the proton case the calculation of the free-gas contribution has included the Coulomb interaction too. This case was chosen especially due to the equal numbers of neutrons and protons of $^{40}$Ca, so that it can be observed the effect of taking into account the both kinds of nucleons. Actually, the comparison of the exact QM and TF approximation is shown in Fig. 5(a) only for neutrons, while next is given the QM calculated contributions of the both systems of nucleons as well as their sum.

V. CONCLUSIONS

A quantum-mechanical calculation of the single-particle level (s.p.l.) density $g(\varepsilon)$ is carried on by using the connection with the single-particle Green’s function. The relation between the imaginary part of Green’s function and single-particle wave functions is used separately for the discrete and continuous states. Within the bound-states region the imaginary part of the Green’s function is calculated by using the wronskian theorem. The Green’s function corresponding to the continuum is written by using the regular and Jost solutions of the radial Schrödinger equation. The smooth part of the rapidly fluctuating s.p.l. density is calculated by means of the Strutinski procedure.

Recently Shlomo [3] calculated the s.p.l. density by using the Green’s function method, the phase-shift approach, and the TF approximation. The following different points could be underlined between the present work and the Shlomo’s analysis. First, the smearing procedure used by Shlomo [4] is replaced with the exact calculation of the imaginary part of the Green’s function carried out distinctively for the both bound and continuum regions of the spectrum. Second, Shlomo has considered the nucleus contained in a large but finite box within both the Green’s function method and the phase-shift approach. This condition is not required in the present work. Third, we have taken into account the case of the protons too, where the Coulomb interaction has to be also included in the contribution of the free gas.

Finally, it results that the continuum component of the s.p.l. density has rather close values within either exact QM calculations with the WS potential, or TF approximation with WS as well as FSQ potential wells, provided that the free-gas contribution is subtracted. A similar trend is obtained by means of the simple FGM formula for the s.p.l. density, if the continuum effect is taken into account. The level of agreement between this phenomenological formula and the QM calculation could be improved for lower values of the Fermi energy $F$ which is usually considered $\sim$38 MeV [1]. It is thus even possible to reproduce the quantum-mechanical results by using the average Fermi energy $\bar{F} \sim$20 MeV [7, 15]. Additional analysis is yet required by, e.g., adoption of realistic mean-field potentials energy dependent [4], and systematic calculations of s.p.l. density including the continuum effect.

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