Semiclassical Calculation of One-Particle, One-Hole and Two-Particle, Two-Hole Level Densities

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One-particle, one-hole and two-particle, two-hole level densities are calculated in the local-density, i.e., Thomas-Fermi, approach. For the harmonic oscillator this leads to analytical expressions which are in excellent agreement with the exact quantum results.

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In a recent work, Schuck, Ghosh, and Hasse[1] have shown how to calculate in Thomas-Fermi approximation the average part of particle-hole (p-h) multipole transition strengths. We here apply the same technique for the evaluation of average 1p-1h and 2p-2h level densities. These quantities obviously are of interest as, for example, in precompound reactions or in the study of the spreading width of giant resonances,[2] to name only a few. On the other hand, it seems appropriate to evaluate those multiparticle-multihole level densities in a statistical model because of the extremely high density of states for excitation energies $\geq \hbar\omega_0$ (a typical shell spacing). The interesting energy range for level densities, however, lies mainly about the Fermi energy. Statistical models for the evaluation of level densities, of course, have been applied long ago[3] but to our knowledge, no attempts have been made to calculate these quantities in a systematic expansion in $\hbar$ [extended Thomas-Fermi (ETF) approach]. This approach has obvious advantages since it takes into account the specific shapes of individual potentials and yields for each potential (e.g., harmonic oscillator, Woods-Saxon, etc.) in a well defined way the average part of the corresponding exact quantity. This has been demonstrated extensively in the past for quantities such as ground-state energies,[4] moments of inertia,[5] pairing energies,[6] etc. In most of these cases, a corresponding Strutinsky calculation exists and perfect agreement between the semiclassical and the Strutinsky approach has always been found.[7] Since some of these quantities involve already 1p-1h states around the Fermi surface (e.g., moment of inertia) it seems natural to apply the ETF approach also to multiparticle, multihole states, and to surmise that the results are the same as would have been obtained from a Strutinsky calculation.

Indeed, in a numerical example for the three-dimensional harmonic oscillator we show below that our semiclassical level densities pass very nicely through the average of the exact ones and we conjecture from the experience one has obtained in the meanwhile with the ETF approach that this will be the same for more general potentials of the Woods-Saxon type.

Our starting points are the definitions for the single-particle, 1p-1h, and 2p-2h level densities:

$$g_{1p}(E)=\sum_k \delta(E-\epsilon_k), \tag{1a}$$

$$g_{1p1h}(E)=\sum_{p,h}\delta(E-\epsilon_p+\epsilon_h), \tag{1b}$$

$$g_{2p2h}(E)=\sum_{p_1<p_2,\,h_1<h_2}\delta(E-\epsilon_{p_1}-\epsilon_{p_2}+\epsilon_{h_1}+\epsilon_{h_2}), \tag{1c}$$

where the ϵ_i are the eigenvalues of the single-particle Hamiltonian H (spherical harmonic oscillator in our case) and the sums go over particles and holes [note that in (1c) the Pauli principle is obeyed;

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the well-known case of the single-particle level density[7] is only treated for the sake of completeness].

We now rewrite (1) in a representation-independent way:

$$g_{1p}(E) = \mathrm{Tr}\,\{\delta(E-H)\}, \tag{2a}$$

$$g_{1p1h}(E) = \mathrm{Tr}_1\,\mathrm{Tr}_2\,\{\theta(\epsilon_F - H_2)\,\theta(H_1-\epsilon_F)\,\delta(E-H_1+H_2)\}, \tag{2b}$$

$$\begin{aligned} g_{2p2h}(E) = {} & \mathrm{Tr}_1\,\mathrm{Tr}_2\,\mathrm{Tr}_3\,\mathrm{Tr}_4\,\{\theta(\epsilon_F-H_4)\,\theta(\epsilon_F-H_3)\,\theta(H_2-\epsilon_F)\,\theta(H_1-\epsilon_F)\,\delta(E-H_1-H_2+H_3+H_4)\} \\ & - \mathrm{Tr}_1\,\mathrm{Tr}_2\,\mathrm{Tr}_3\,\{\theta(\epsilon_F-H_3)\,\theta(H_1-\epsilon_F)\,\theta(H_2-\epsilon_F)\,\delta(E-H_1-H_2+2H_3)\} \\ & - \mathrm{Tr}_1\,\mathrm{Tr}_2\,\mathrm{Tr}_3\,\{\theta(\epsilon_F-H_3)\,\theta(\epsilon_F-H_2)\,\theta(H_1-\epsilon_F)\,\delta(E-2H_1+H_2+H_3)\} \\ & + \mathrm{Tr}_1\,\mathrm{Tr}_2\,\{\theta(\epsilon_F-H_2)\,\theta(H_1-\epsilon_F)\,\delta(E-2H_1+2H_2)\}, \end{aligned} \tag{2c}$$

where $\theta(x)$ stands for the unit step function. It is straightforward to proceed from (2) to the Thomas-Fermi approximation,[7] i.e., replacing the operators H_i by their classical counterparts,

$$H_i{}^c = p_i{}^2/2m + V(\boldsymbol{r}_i), \tag{3}$$

and the traces by integrations over phase space,

$$\mathrm{Tr}_i \to n_i \int (2\pi\hbar)^{-3} d^3r_i\, d^3p_i, \tag{4}$$

where n_i denotes the spin-isospin degeneracy.

For the special case of the spherical harmonic oscillator $V = m\omega_0{}^2r^2/2$, we can perform the integration analytically and we obtain the results (without $\hbar$ corrections and with spin but without isospin factors)

$$\hbar\omega_0 g_{1p}{}^{TF}(E) = \epsilon^2, \tag{5a}$$

$$\hbar\omega_0 g_{1p1h}{}^{TF}(E) = \frac{\lambda^4\epsilon}{2} + \frac{\epsilon^5}{60} - \frac{(\epsilon-\lambda)^3}{6}\,\theta(\epsilon-\lambda)\left[\lambda^2 + \frac{\lambda(\epsilon-\lambda)}{2} + \frac{(\epsilon-\lambda)^2}{10}\right], \tag{5b}$$

$$\begin{aligned} \hbar\omega_0 g_{2p2h}{}^{TF}(E) = {} & \frac{\epsilon}{16}\left[\frac{\lambda^8\epsilon^2}{3!} + \frac{8\lambda^4\epsilon^6}{7!} + \frac{16\epsilon^{10}}{11!} - \lambda^6\epsilon - \frac{9\lambda^4\epsilon^3}{4!} - \frac{4\epsilon^7}{8!} + \lambda^4 + \frac{\epsilon^4}{4\times 5!}\right] \\ & - \frac{(\epsilon-\lambda)^4}{4}\,\theta(\epsilon-\lambda)\left[\frac{\lambda^6(\epsilon-\lambda)}{5!} + \frac{2\lambda^5(\epsilon-\lambda)^2}{6!} + \frac{2\lambda^4(\epsilon-\lambda)^3}{7!} + \frac{4\lambda^2(\epsilon-\lambda)^5}{9!} + \frac{8\lambda(\epsilon-\lambda)^6}{10!} + \frac{8(\epsilon-\lambda)^7}{11!}\right. \\ & \left. - \frac{\lambda^4}{4!} + \frac{\lambda^3(\epsilon-\lambda)}{5!} - \frac{\lambda^2(\epsilon-\lambda)^2}{2\times 6!} - \frac{\lambda(\epsilon-\lambda)^3}{7!} - \frac{(\epsilon-\lambda)^4}{8!}\right] \\ & + \frac{(\epsilon-2\lambda)^3}{4}\,\theta(\epsilon-2\lambda)\left[\frac{\lambda^4(\epsilon-2\lambda)^4}{7!} + \frac{4\lambda^3(\epsilon-2\lambda)^5}{8!} + \frac{8\lambda^2(\epsilon-2\lambda)^6}{9!} + \frac{8\lambda(\epsilon-2\lambda)^7}{10!} + \frac{4(\epsilon-2\lambda)^8}{11!}\right. \\ & \left. + \frac{\lambda^4(\epsilon-2\lambda)}{8\times 4!} + \frac{\lambda^3(\epsilon-2\lambda)^2}{2\times 5!} - \frac{\lambda^2}{8\times 3!} - \frac{\lambda(\epsilon-2\lambda)}{8\times 4!} - \frac{(\epsilon-2\lambda)^2}{16\times 5!}\right]. \end{aligned} \tag{5c}$$

Here, $\epsilon = E/\hbar\omega_0$, and $\lambda = \epsilon_F/\hbar\omega_0$ follows from number conservation in lowest order of $\hbar$[7]:

$$\lambda = (3N)^{1/3}. \tag{6}$$

For the harmonic oscillator, one can also evaluate the exact quantum level densities from combinatorics:

$$\hbar\omega_0 g_{1p}{}^{QM}(E) = \sum_{n=1}^{\infty} \delta(\epsilon - n - \tfrac{1}{2})\,n(n+1), \tag{7a}$$

$$\hbar\omega_0 g_{1p1h}{}^{QM}(E) = \frac{1}{2}\sum_{n=1}^{\infty}\delta(\epsilon-n) \sum_{\substack{1\le i\le \lambda' \\ \lambda'+1\le m\le \lambda'+n \\ m-i=n}} i(i+1)m(m+1), \tag{7b}$$

$$\hbar\omega_0 g_{2p2h}{}^{QM}(E) = \frac{1}{4}\sum_{n=1}^{\infty}\delta(\epsilon-n) \sum_{\substack{1\le i,j\le \lambda' \\ \lambda'+1\le m,k\le \lambda'+n \\ m+k-i-j=n}} i(i+1)\left(\frac{j(j+1)}{2} - \delta_{ij}\right) m(m+1)\left(\frac{k(k+1)}{2} - \delta_{mk}\right). \tag{7c}$$

Here, the Fermi energy follows from

$$\lambda'^3 + 2\lambda'^2 + 2\lambda' = 2N. \quad (8)$$

The sums (7) can be performed analytically but the expressions become too lengthy to be shown here.

In order to compare our semiclassical expressions which represent average quantities to the exact quantum mechanical ones which are a succession of δ peaks, we display in Fig. 1 for the low-energy part the integrated quantities

$$N_{1p,1p1h,2p2h}(E) = \int_0^E dE' g_{1p,1p1h,2p2h}(E'), \quad (9)$$

i.e., the corresponding number of states. From this figure one sees how precisely the Thomas-Fermi result passes through the average of the steplike exact functions. In looking, however, very closely, one sees that our results are slightly above average, a feature which can certainly be cured in evaluating the $\hbar^2$ correction to the above result; this is straightforward, but tedious to do. The effect can be studied nicely in the well-known and very simple case of the one-particle level density or the number of particles which reads, with $\hbar^2$ corrections,[7]

$$N_{1p}{}^{TF}(E) = \tfrac{1}{3}\epsilon^3 - \tfrac{1}{4}\epsilon. \quad (10)$$

Here, the second term lowers the zero-order result by a very small amount, just enough to bring it precisely to the average. The level densities are displayed in Fig. 2, where the dots represent the height of rectangles with unit base whose areas are equal to the weights of the corresponding δ peaks. We thus achieve a gross averaging of the exact level density which is to be compared with our semiclassical result.

We would like to point out that besides the excellent overall agreement of the semiclassical results with the exact ones even such fine details as the small number of 2p-2h states for $0 \leq E/\hbar\omega_0 \lesssim 2$ (Fig. 1) and the discontinuity of the derivatives of the level densities around the Fermi level are reproduced semiclassically.

One also observes that for large energies the Thomas-Fermi level densities are asymptotically exact. For excitation energies high above the Fermi level our harmonic oscillator model is, of course, inadequate and Fig. 2 in this range only serves for comparison of our Thomas-Fermi approach with the exact level densities. For finite potentials the energy range which corresponds to excitations into the continuum has to be treated with extra care.[8] Finally we note that $g_{1p1h}{}^{TF}$ of Eq. (5),

$$g_{1p1h}{}^{TF}(E) = g_0{}^2 E(1 + E^4/30\epsilon_F{}^4), \quad E \leq \epsilon_F, \quad (11)$$

where $g_0 = \epsilon_F{}^2/(\hbar\omega_0)^3 = 3N/\epsilon_F$ is the single-particle level density at the Fermi energy, represents an improved version of Ericson's formula,[3] now valid for all energies below the Fermi energy.

For a Woods-Saxon potential, the integrations involved in (2) and (4) have to be performed numerically but as mentioned above there are strong reasons to believe that the results compare as favorably with the exact ones as in the harmonic-oscillator case. This belief stems from other studies[4] within the ETF formalism where the accuracy of the results is independent of the potential. We hope to present calculations with a Woods-Saxon potential together with a more elaborate version of the paper elsewhere.

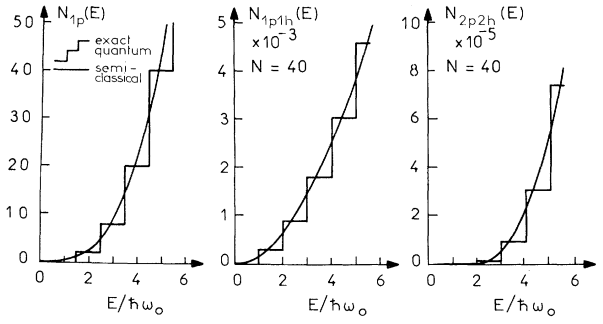

FIG. 1. Single-particle; one-particle, one-hole; and two-particle, two-hole numbers of states in the Thomas-Fermi approximation and calculated quantum mechanically.

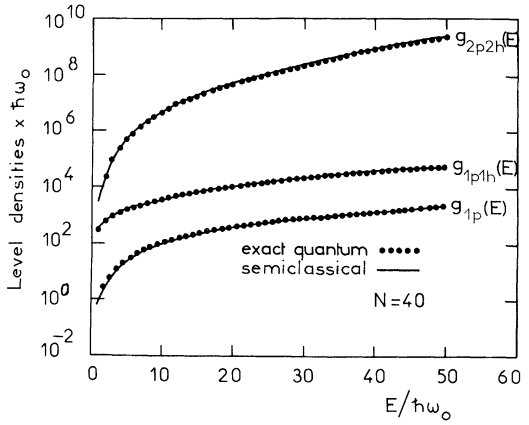

FIG. 2. Same as Fig. 1 but level densities. The dots represent the heights of rectangles with unit base whose areas are equal to the weights of the corresponding δ peaks.

For 2p-2h states which enter the width of giant resonances we have to project onto good angular momentum. Also this can be done successfully within the Thomas-Fermi approach as we have demonstrated in our preceding paper[1] on the quadrupole p-h transition strength.

In conclusion, we have demonstrated here how multiparticle, multihole level densities can be calculated very accurately within the Thomas-Fermi approach. In spite of its great simplicity we are not aware of any earlier attempts in this direction and we thus think that our novel method may be quite promising for problems where these level densities are of importance. As a first application we are presently trying to evaluate the spreading width of giant resonances (2p-2h states)[2] within this formalism. But other quantities such as, for example, the imaginary part of the nucleon optical potential (2p-1h states) are certainly equally interesting.

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