Effective Mass and Excitation of Nuclei

Toshio SUZUKI

Research Institute for Fundamental Physics
Kyoto University, Kyoto 606

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It is discussed how the effective mass, \( m^* \), manifests in the calculation of various energies in the Hartree-Fock field, by using the Skyrme force. Whereas the average spacing between occupied major shells and the mean excitation energy of quasielastic scattering are scaled as \( m/m^* \), excitation energies for dipole and quadrupole modes show different \( m^* \)-dependences due to nuclear surface effects.

§ 1. Introduction

More than ten years ago, Gillet and Brown et al.\(^{1}\) pointed out that RPA calculations yield excitation energies of dipole states not to be high enough to reproduce experimental values, in spite of using reasonable effective interactions and empirical single-particle energies, \( \omega_0 \approx 41/A^{1/3} \) (MeV) as unperturbed ones. For the long-standing problem, recently, Brown et al.\(^{2}\) argued that in discussing high lying nuclear vibrations one should use the unperturbed energies, \( \omega \), corresponding to the effective mass, \( m^* (< m) \), instead of \( \omega_0 \) determined for the free nucleon mass, \( m \). Since one may obtain the value of \( \omega \) to be higher than \( \omega_0 \), a part of the discrepancy might be resolved. Then, Brown et al.\(^{2}\) have proposed to use \( \omega = \omega_0 (m/m^*) \) as unperturbed energies of dipole excitations.

It has been also discussed by many authors\(^{3-6}\) that the effective mass plays an important role in excitation energies of quadrupole resonance states. For the arguments in a harmonic oscillator potential model, Bohr and Mottelson\(^{3}\) used the same \( m^* \)-dependence as \( \omega = \omega_0 (m/m^*) \). The scaling factor \( (m/m^*) \) is obtained by adjusting the oscillator frequency so as to retain the spatial dimension, \( \langle r^2 \rangle \), in a harmonic oscillator potential model.\(^{3,5}\)

The purpose of the present paper is to study in more detail the dependence of excitation energies of various modes on the effective mass, \( m^* \), using explicitly the Hartree-Fock potential given by the Skyrme forces.\(^{7,8}\) We will show that the average spacing between occupied major shells and the mean excitation energy of quasielastic electron scattering\(^{9}\) in the Hartree-Fock field are scaled with \( m/m^* \), as in the previous models, but that excitation energies for dipole and quadrupole modes have different \( m^* \)-dependences because of surface effects.

In the following section we will briefly review the Skyrme forces, and in § 3, \( m^* \)-dependence of various energies will be discussed. The final section is devoted
to a summary of this paper.

§ 2. Skyrme forces

The Skyrme force neglecting the spin-orbit force is written as

\[ V = \sum_{i\neq j} v_{ij} + \sum_{i\neq j\neq k} v_{ijk} \] (1)

with

\[ v_{ij} = t_0(1 + x_0 P^\sigma) \delta(r_i - r_j) \]
\[ + \frac{1}{2} t_1 [\delta(r_i - r_j) k^2 + k^2 \delta(r_i - r_j)] + t_2 k \cdot \delta(r_i - r_j), \]
\[ (P^\sigma = (1 + \sigma(i) \cdot \sigma(j))/2, \quad k = (p_i - p_j)/2) \]
\[ v_{ijk} = t_3 \delta(r_i - r_j) \delta(r_j - r_k). \]

Then, the Hartree-Fock Hamiltonian for \( N = Z \) nuclei is given by

\[ H_{H.F.} = T + U, \] (2)

where the kinetic part is described as

\[ T = -\nabla \cdot \frac{1}{2m^*(r)} \nabla \] (\( \hbar = 1 \))

with the effective mass \( m^*(r) \):

\[ m/m^*(r) = 1 + \frac{1}{8}(3t_1 + 5t_2) m \rho_0(r), \] (4)

and the potential part is

\[ U = \left\{ \frac{3}{4} t_0 + \frac{3}{16} t_3 \rho_0(r) \right\} \rho_0(r) \]
\[ + \frac{1}{16} (3t_1 + 5t_2) \tau_0(r) + \frac{1}{32} (5t_2 - 9t_1) P^2 \rho_0(r). \] (5)

Here, the density, \( \rho_0(r) \), and the kinetic energy density, \( \tau_0(r) \), of the ground state have been defined by

\[ \rho_0(r) = \sum_{i=1}^A |\phi_i^0(r)|^2, \]
\[ \tau_0(r) = \sum_{i=1}^A \nabla \phi_i^0(r) \cdot \nabla \phi_i^0(r), \]

\( \phi_i^0(r) \) being an eigenfunction of Eq. (2) with the single-particle energy, \( \varepsilon_i \). The effective mass, \( m^*(r) \), comes from the velocity-dependent parts of the Skyrme force as in Eq. (4). In nuclear matter, \( \rho_0(r) = \rho_0 = 0.17/\text{fm}^3 \), it is written as
\[ m = \frac{1}{m^*} = 1 + \frac{1}{8} (3t_1 + 5t_2) m \rho_0. \]  

(6)

§ 3. \( m^* \) dependence

3.1. Single-particle energies of occupied states

First, we estimate the average spacing between occupied major shells by calculating \( \sum \varepsilon_i \),

\[ \sum_{i=1}^{A} \varepsilon_i = \langle T \rangle_0 + \langle U \rangle_0, \]  

(7)

where

\[ \langle T \rangle_0 = \int \frac{1}{2m^* r} \tau_0(r) dr - \frac{1}{2m^*} \int \tau_0(r) dr, \]  

(8)

\[ \langle U \rangle_0 = \int \left\{ \frac{3}{4} t_0 + \frac{3}{16} t_2 \rho_0(r) \right\} \rho_0^2(r) dr \]

\[ + \frac{1}{16} (3t_1 + 5t_2) \int \tau_0(r) \rho_0(r) dr \]

\[ + \frac{1}{32} (5t_3 + 9t_1) \int \rho_0(r) V^2 \rho_0(r) dr. \]  

(9)

Neglecting the surface term of Eq. (9) and assuming the \( t_1 \)- and \( t_2 \)-independent part of \( U \) to be replaced by a harmonic oscillator potential with \( \omega_0 \),

\[ \left\{ \frac{3}{4} t_0 + \frac{3}{16} t_2 \rho_0(r) \right\} \rho_0(r) \approx - V_0(\text{constant}) + \frac{\omega_0^2}{2} r^2, \]

\[ (\omega_0 = 41/A^{1/3} \text{ (MeV)}) \]  

(10)

Eq. (9) is written as

\[ \langle U \rangle_0 \approx - V_0 A + \int \frac{\omega^2}{2} \rho_0^2(r) dr + \frac{1}{16} (3t_1 + 5t_2) \rho_0 \int \tau_0(r) dr \]

\[ \approx - V_0 A + \frac{m}{m^*} \int \frac{\omega^2}{2} r^2 \rho_0(r) dr. \]  

(11)

In the last step of Eq. (11), we have utilized the approximation,

\[ \int \frac{\omega^2}{2} r^2 \rho_0(r) dr = \frac{1}{2m} \int \tau_0(r) dr, \]  

(12)

which is valid in a harmonic oscillator potential model. Inserting Eqs. (8) and (11) into Eq. (7) leads finally to

\[ \sum_{i=1}^{A} \varepsilon_i \approx \frac{1}{2m^*} \int \tau_0(r) dr - V_0 A + \frac{m}{m^*} \int \frac{\omega^2}{2} r^2 \rho_0(r) dr. \]  

(13)
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which is equal to that obtained from the Hamiltonian,

\[ H = \frac{1}{2m^*} \sum_{i=1}^{A} p_i^2 + AV_0 + \sum_{i=1}^{A} \frac{m^* \omega^2}{2} r_i^2. \]  

(14)

with a harmonic oscillator constant, \( \omega \),

\[ \omega = \left( \frac{m}{m^*} \right) \omega_0. \]  

(15)

Thus, the average spacing between occupied major shells, \( \omega_0 \), is scaled as \( (m/m^*) \) due to the velocity-dependent forces, and the scaling factor is the same as that used by Bohr and Mottelson\(^{30}\) and Brown et al.\(^{23}\) Their derivation of the factor is based on retaining the spatial dimension by \( \langle r^2 \rangle \sim 1/m \omega_0 = 1/m^* \omega \), but our argument includes further assumptions.

Next, we study whether or not one can use Eq. (14) to estimate excitation energies.

3.2. Dipole excitations

We perform the time-dependent gauge and the scale transformation of \( \phi_i^q(r) \) \( (i=1, \cdots A) \)

\[ \phi_i(r) = e^{im\xi(r,t)} \phi_i^q(x, y, z + \nu(t)) \]  

(16)

and construct a Slater determinant \( |\Phi\rangle \) with the set \( \{ \phi_i(r) \} \) \( (i=1, \cdots A) \) to describe dipole motions.\(^{4,6,10,11}\) The relationship between the velocity field \( \xi \) and the collective variable \( \nu \) is determined by the continuity equation,

\[ \frac{\partial}{\partial t} \langle \Phi | \dot{\rho} (r) | \Phi \rangle = i \langle \Phi | [H_{\text{HF}}, \ \dot{\rho} (r)] | \Phi \rangle = -\nabla \cdot \left[ \left\{ 1 + \frac{1}{8} (3t_1 + 5t_2) m \omega_0 (r) \right\} \rho (r) \nabla \frac{\xi}{m} \right] \]

(17)

for the density

\[ \langle \Phi | \dot{\rho} (r) | \Phi \rangle = \rho_0 (x, y, z + \nu(t)) = \rho (r), \]  

(18)

which yields

\[ \xi (r, t) \approx -\frac{m}{m^*} \frac{\nu}{z}. \]  

(19)

The expectation value of \( H_{\text{HF}} \) is easily calculated and expanded up to \( O(\nu^2) \),

\[ \langle \Phi | T + U | \Phi \rangle \approx \langle T + U \rangle_0 + \frac{m^* A}{2} \nu^2. \]
where we have neglected a small contribution from the last term of Eq. (5) and used the relationship, Eq. (19). First, let us consider the second and the third term of Eq. (20) leaving out the fourth term. Then, in using the approximation, Eq. (10), Eq. (20) is expressed as

\[ \langle \Phi | H | \Phi \rangle = \langle T + U \rangle + \frac{m^* A}{2} \nu^2 + \frac{m}{2} \omega_0^2 \nu^2, \]  

yielding the excitation energy, \( \omega_1 \), for dipole excitations,

\[ \omega_1 = \sqrt{m/m^*} \omega_0. \]  

If the fourth term of Eq. (20) were expressed approximately as \( \nu^2 / 2 \times (3t_1 + 5t_2) \rho_0 m \omega_0 A \nu^2 \), Eq. (22) would become \( \omega_1 = \omega_0 m/m^* \) as in Eq. (15). However, its contribution to the excitation energy is not simply expressed in terms of \( m^* \) for nuclear matter, since the integral is due to the surface effect.

Moreover, this yields a negative contribution. Thus \( \omega_1 \) is not simply scaled as \( \omega_0 m/m^* \).

It should be noted that the scaling factor \( \sqrt{m/m^*} \) in Eq. (22) stems from the mass parameter, \( m^* A \), as seen in Eq. (21). Therefore, if we take account of the residual forces depending on \( t_1 \) and \( t_2 \), in addition to \( H_{\text{F,F}} \), it must be replaced by \( \sqrt{1+x} \) (Refs. 3, 6, 11, 12), \( x \) denoting the increment of the classical energy-weighted sum-rule value for dipole excitations.

\[ x = \begin{cases} 0 & \text{for isoscalar modes}, \\ \frac{1}{2} (t_1 + t_2) \rho_0 & \text{for isovector modes}. \end{cases} \]  

3.3. Quadrupole excitations

For quadrupole excitations, we perform the following transformation of single-particle wave functions \( \phi_i^0(r)(i = 1, \cdots A) \) (Refs. 4, 6, 10, 11)

\[ \phi_i(r) = e^{im\xi(r,t)} e^{-\mu(t)x, e^{-\mu(t)y}, e^{3\mu(t)z}}. \]  

The relationship between \( \xi \) and \( \nu \) is obtained as
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\[ \xi(r, t) = -\frac{m^*}{m} \frac{1}{2} \sqrt{\frac{16\pi}{5}} r Y_{20}(\hat{r}) \psi \]  

by using the continuity equation Eq. (17) and

\[ \langle \Phi | \hat{\rho}(r) | \Phi \rangle = \rho_0(e^{-\nu x}, e^{-\nu y}, e^{i\nu z}) = \rho(r), \]

where |\Phi\rangle stands for a single determinant composed of \( \phi_i(r)(i = 1, \ldots, A) \). For the transformed wave function, we have the expectation value of \( H_{\text{ex}}, \) neglecting the third term of \( U \),

\[ \langle \Phi | T + U | \Phi \rangle = \langle T + U \rangle_0 + \frac{1}{2} 2 m^* A \langle \nu^2 \rangle \rho_0 + 4 \nu^2 m^* \frac{1}{2 m} \int \tau_0(r) dr \]

\[ + \frac{\nu^2}{2} \int \left[ \frac{3}{4} t_0 + \frac{3}{16} t \rho_0(r) \right] \rho_0(r) \rho_0(r) dr \]

\[ + \frac{\nu^2}{2} \frac{1}{8} \left( 3 t_1 + 5 t_2 \right) \int \phi_0(r) \rho_2(r) dr \]

\[ + 2 \int \rho_1(r) (2 \tau_0^x - \tau_0^x - \tau_0^x) dr \],

where we have defined

\[ \rho_1(r) = \sqrt{\frac{16\pi}{5}} r \frac{d \rho_0(r)}{dr} Y_{20}, \quad \rho_2(r) = \frac{4}{5} r^2 \frac{d}{dr} \left( r \frac{d \rho_0(r)}{dr} \right) \]

and

\[ \tau_0^x(r) = \sum_{\overline{1}} \nabla \chi \phi_i^*(r) \nabla \chi \phi_i^0(r), \quad \text{etc.} \]

The third term of Eq. (27), which is a volume term, comes from the distortion of the kinetic energy density, and has been obtained by the approximation,

\[ 4 \nu^2 \frac{1}{2 m} \int \tau_0(r) dr + 4 \nu^2 \frac{1}{8} (3 t_1 + 5 t_2) m^* \frac{1}{2 m} \int \rho_0(r) \tau_0(r) dr \]

\[ \approx 4 \nu^2 \frac{m^*}{m} \frac{1}{2 m} \int \tau_0(r) dr . \]

The fourth term of Eq. (27) arises from the breaking of the self-consistency between the Hartree-Fock field and the vibrating density near the nuclear surface. If we use the approximation Eqs. (10) and (12), the third and the fourth term of Eq. (27) are expressed as

\[ 4 \nu^2 \frac{m^*}{m} \frac{1}{2 m} \int \tau_0(r) dr = \nu^2 \cdot 2 m A \langle \nu^2 \rangle \cdot \frac{m^*}{m^*} \cdot 2 \omega^2 , \]

\[ \frac{\nu^2}{2} \int \left[ \frac{3}{4} t_0 + \frac{3}{16} t \rho_0(r) \right] \rho_0(r) \rho_2(r) dr = \frac{\nu^2}{2} \cdot 2 m A \langle \nu^2 \rangle \cdot 2 \omega^2 . \]
Therefore, leaving the last term of Eq. (27) out, Eqs. (27), (29) and (30) give the unperturbed energy, \( \omega_s \), for quadrupole excitations,

\[
\omega_s = \left\{ \left( \frac{m}{m^*} \right)^2 2 \omega_0 + \left( \frac{m}{m^*} \right)^2 \omega_0^2 \right\}^{1/2}.
\] (31)

This becomes \( 2 \omega_0 \) for \( m^* = m \) as expected in a harmonic oscillator model, but is scaled in a different way from \( 2 \omega_0 m/m^* \) in Eq. (15). The first term in the brackets has the same scaling factor as that in Eq. (15), while the second term is scaled as in Eq. (22) for dipole modes. This reflects the fact that the former is obtained from the integral to which the whole volume contributes, whereas the latter from the nuclear surface effect. The last term of Eq. (27), that is, the effect of the velocity-dependent forces near the nuclear surface is not simply expressed by using \( m^* \).

As seen in Eq. (27), the mass parameter for the quadrupole excitation in \( H_{\text{rel}} \) is given by \( 2m^* A \langle r^2 \rangle \). If we take account of the residual forces depending on \( t_1 \) and \( t_2 \), it reduces to \( 2m A \langle r^2 \rangle \) for isoscalar modes (IS) and to \( 2mA \langle r^2 \rangle/(1+x) \) for isovector modes (IV) (Refs. 3, 6)). Therefore, Eq. (31) becomes \( \{(m/m^*)^2 \omega_0^2 + 2 \omega_0^2 \}^{1/2} \) for IS and \( \{((m/m^*)^2 \omega_0^2 + 2 \omega_0^2) (1+x) \}^{1/2} \) for IV. It is known that other residual forces cancel \( 2 \omega_0^2 \)-term in IS, to have finally the excitation energy for isoscalar modes, \( \{(m/m^*)^2 \omega_0^2 \}^{1/2} \) (Refs. 3, 4)). On the other hand, in IV, \( 2 \omega_0^2 \)-term remains as it is, and the further contribution, \( \Delta_{\text{sym}} \), from the symmetry potential appears as \( \{(m/m^*)^2 \omega_0^2 + 2 \omega_0^2 + \Delta_{\text{sym}} (1-x) \}^{1/2} \) (Ref. 6)). The surface effect of the \( t_1 \) - and \( t_2 \)-forces, like the last term of Eq. (27), also remains in IV, but with the factor, \( (t_1 + t_2) \), instead of \( (3t_1 + 5t_2) \).

3.4. Quasielastic scattering

Although we should not use the Skyrme forces for the argument of excitations by high-momentum transfer, it is instructive for our purpose to discuss quasielastic scattering of electrons\(^9\) with use of them. We define the mean energy, \( \bar{\omega} \), of the excitations by

\[
\bar{\omega} = S_1/S_0,
\] (32)

where

\[
S_0 = \sum_n \left| \langle n| \sum_{k=1}^A e^{iqr_0} (1 + r_0(k)) |0 \rangle \right|^2
\] (33)

and

\[
S_1 = \sum_n (E_n - E_0) \left| \langle n| \sum_{k=1}^A e^{iqr_0} (1 + r_0(k)) |0 \rangle \right|^2,
\] (34)

\( q \) standing for the momentum transfer from the electron to the nucleus. In the Fermi gas model, \( S_0 \) and what is called \( f \)-sum rule, \( S_1 \), are given by\(^{10}\)}
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\[ S_0 = Z, \quad (q > 2k_F) \]  \hfill (35)

\[ S_i = \frac{q^2}{2m^*} Z, \]  \hfill (36)

where \( k_F \) denotes the Fermi momentum. Hence, we have the well-known mean energy, \( \bar{\omega}_F \), corresponding to the peak position of the response function.\(^9\)

\[ \bar{\omega}_F = \frac{q^2}{2m}, \quad (q > 2k_F) \]  \hfill (37)

Now, when the nuclear Hamiltonian is given by Eq. (2), \( S_i \) is evaluated to be

\[ S_i = \frac{q^2}{2m^*} Z \cdot \frac{m^*}{m^*}. \]  \hfill (38)

Since \( S_0 \) is given by Eq. (35) as \( q \to \infty \) even for the Hamiltonian, Eq. (2), we have the mean energy, \( \bar{\omega} \),

\[ \bar{\omega} = \bar{\omega}_F \cdot \frac{m^*}{m^*}. \]  \hfill (39)

Thus, the peak-energy is scaled as \( m/m^* \) due to the effective mass, as in Eq. (15). In the previous subsections, we have obtained the scaling factor \( m/m^* \), if the energies considered come from the volume effects. The present result, Eq. (39), is also due to a kind of the volume effect, since in quasielastic scattering with high \( q > 2k_F \), all nucleons in the nucleus can contribute to the process.

It should be noted, however, that in taking the residual interactions in addition to Eq. (2), \( S_i \) is given by \( q^2 Z(1+x)/2m \), and, therefore, we have \( \bar{\omega} = \bar{\omega}_F (1 + x) \). This fact means that one cannot extract \( m^* \) directly, but \( x \) from experimental values of the displacement energy of the peak position from \( \bar{\omega}_F \) in quasielastic scattering.\(^{14,15}\) In Skyrme forces, \( x \) is given by \( (t_1 + t_2) m \bar{\rho}_0/2 \), but in more realistic nuclear forces with finite range, \( x \) shows the \( q \)-dependence, and, in the limit \( q \to 0 \), is related to \( x \) for isovector dipole excitations.\(^{15}\)

§ 4. Summary

By using the Skyrme forces, we have studied how the effective mass, \( m^* \), appears in the calculation of various energies in the Hartree-Fock field. It is shown that whereas the energies coming from the volume effect are scaled as \( m/m^* \), the ones due to the nuclear surface effect are as \( \sqrt{m/m^*} \). The average spacing between occupied major shells and the mean excitation energy of quasielastic scattering in the Hartree-Fock field are examples of those scaled by \( m/m^* \). In dipole excitations, on the other hand, the restoring force is due to the surface effect and, therefore, the excitation energy is scaled as \( \sqrt{m/m^*} \). The
restoring force for quadrupole excitations stems from both the volume and the surface effect. As a result, the excitation energy of quadrupole modes is scaled as in Eq. (31). The velocity-dependent forces yield another contribution to the restoring forces for dipole and quadrupole modes as a surface effect which is not expressed in terms of \( m^* \) for nuclear matter.

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