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To cite this article: Wen-Chao Qiang and Shi-Hai Dong 2010 *EPL* **89** 10003

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Proper quantization rule

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received 28 September 2009; accepted in final form 7 December 2009

published online 4 January 2010

PACS 03.65.Fd – Algebraic methods

PACS 34.20.Cf – Interatomic potentials and forces

PACS 03.65.Ta – Foundations of quantum mechanics; measurement theory

Abstract – We find a proper quantization rule, $\int_{x_A}^{x_B} k(x)dx - \int_{x_{0A}}^{x_{0B}} k_0(x)dx = n\pi$, where n is the number of the nodes of wave function $\psi(x)$. By this rule the energy spectra of a solvable system can be determined from its ground-state energy only. Particularly, we study three solvable quantum systems —modified Rosen-Morse potential, symmetric trigonometric Rosen-Morse potential and Manning-Rosen potential in D dimensions— with the proper quantization rule, and show that the previous complicated and tedious calculations can be greatly simplified. This proper quantization rule applies to any exactly solvable potential, and one can easily obtain its energy spectra with the rule.

This work is dedicated to Professor Zhong-Qi Ma on the occasion of his 70th birthday.

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Introduction. – Finding the exact solutions of quantum systems has been an important research subject and attracted much attention in the development of quantum mechanics since they contain all necessary information of the quantum systems. Up to now, several main approaches have been developed to exactly solve quantum systems. They include the SUSYQM approach [1], the Nikiforov-Uvarov method [2], factorization formalism [3] and exact quantization rule method [4,5]. The latter is the generalization of the Bohr-Sommerfeld quantization rule [6] and the WKB approximation [7], which are widely applied to periodic potential, spin system and Gross-Pitaevskii equation [8–11].

The exact quantization rule method is a powerful tool in finding the eigenvalues of all solvable quantum systems [12–17]. It involves complicated integral calculations. Here we improve the method with a considerable simplification for the calculations. This is realized by finding a proper form of the exact quantization rule.

Preliminary. – We begin with a brief review of the exact quantization rule. A one-dimensional Schrödinger equation can be written as a Riccati equation

$$\frac{d}{dx}\phi(x) = -\frac{2\mu}{\hbar^2}[E - V(x)] - \phi(x)^2, \quad (1)$$

where $\phi(x) = \psi(x)^{-1}d\psi(x)/dx$ is the logarithmic derivative of the wave function $\psi(x)$. According to the Sturm-Liouville theorem we know that, between two turning points, $\phi(x)$ decreases monotonically with the increasing x in the region where $E \geq V(x)$. Specifically, as x goes up across a node of the wave function $\psi(x)$, where $E \geq V(x)$, $\phi(x)$ will decrease to $-\infty$, and jump to $+\infty$, and finally decrease again. By carefully studying one-dimensional Schrödinger equation, Ma and Xu proposed an exact quantization rule [4]

$$\int_{x_A}^{x_B} k(x)dx = N\pi + \int_{x_A}^{x_B} k'(x) \frac{\phi(x)}{\phi'(x)} dx, \quad (2)$$

where $k(x) = \sqrt{2M[E - V(x)]}/\hbar$, x_A and x_B two turning points determined by $E = V(x)$. $N = n + 1$ is the number of the nodes of the $\phi(x)$ in the region $E \geq V(x)$, and is larger by one than the number n of the nodes of wave function $\psi(x)$. From now on, we denote the prime, such as $k'(x)$ and $\phi'(x)$ in the above equation, as the first derivative with respect to the argument. The first term $N\pi$ is the contribution from the nodes of the logarithmic derivative of wave function, and the second is called the quantum correction. The authors of ref. [4] found that, for all well-known exactly solvable quantum systems, this quantum correction is independent of the number of nodes

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of wave function. Accordingly, it is enough to consider the ground state in calculating the quantum correction $Q_0 = \int_{x_A}^{x_B} k'_0(x) \frac{\phi_0(x)}{\phi'_0(x)} dx$.

This methodology can be easily extended to D dimensional space. As shown in [17], the effective potential in D dimensions is given by

$$V_{\text{eff.}}(r) = V(r) + \frac{\ell'(\ell' + 1)}{r^2}, \quad \ell' = \left(\ell + \frac{D-3}{2} \right). \quad (3)$$

Thus, the quantization rule

$$\int_{r_A}^{r_B} k(r) dr = N\pi + \int_{r_A}^{r_B} k'_0(r) \frac{\phi_0(r)}{\phi'_0(r)} dr, \quad (4)$$

$$k(r) = \sqrt{2\mu[E - V_{\text{eff.}}(r)]/\hbar}, \quad E \geq V_{\text{eff.}}(r),$$

is still valid for the Schrödinger equation with a spherically symmetric potential in D dimensions.

Proper quantization rule. – There are two integrals in eqs. (2) and (4). In particular, the calculation of the quantum correction term could be very difficult and tedious for some physical potentials. We here improve this method and find its proper quantization rule. To this end, we notice that taking $N = 1$, *i.e.* $n = 0$ in eq. (2) yields

$$\int_{x_{0A}}^{x_{0B}} k_0(x) dx = \pi + \int_{x_{0A}}^{x_{0B}} k'_0(x) \frac{\phi_0(x)}{\phi'_0(x)} dx, \quad (5)$$

$$k_0(x) = \sqrt{2\mu[E_0 - V(x)]/\hbar}.$$

Then the complicated quantum correction will become

$$\int_{x_{0A}}^{x_{0B}} k'_0(x) \frac{\phi_0(x)}{\phi'_0(x)} dx = \int_{x_{0A}}^{x_{0B}} k_0(x) dx - \pi. \quad (6)$$

After substituting this into eq. (2), we obtain

$$\int_{x_A}^{x_B} k(x) dx - \int_{x_{0A}}^{x_{0B}} k_0(x) dx = (N-1)\pi = n\pi. \quad (7)$$

Similarly, eq. (4) can also be written in the same form

$$\int_{r_A}^{r_B} k(r) dr - \int_{r_{0A}}^{r_{0B}} k_0(r) dr = n\pi. \quad (8)$$

Equations (7) and (8) are called the proper quantization rules. The two integrals involved in the proper quantization rule have the same mathematical form. Accordingly, when applying it to calculate the energy levels we can calculate its first integral with respect to $k(x)$ or $k(r)$, and then replace energy levels E_n in the result by the ground-state energy E_0 to obtain the second integral. This will greatly simplify the complicated calculations encountered previously [4,5,12–17].

Applications. – To show the advantage of this proper quantization rule, we shall calculate the eigenvalues of the modified Rosen-Morse potential [15], symmetric trigonometric Rosen-Morse potential [16] and Manning-Rosen

potential in D dimensions. The modified Rosen-Morse potential is given by [15]

$$V(x) = -\frac{U_0 - U_1 \sinh(x/a)}{\cosh^2(x/a)}. \quad (9)$$

With $y = \sinh(x/a)$, the potential is rewritten as

$$V(y) = -\frac{U_0 - U_1 y}{1 + y^2}. \quad (10)$$

Gu *et al.* [15] found the ground-state energy by solving the non-linear Riccati equation (1):

$$E_0 = -\frac{\hbar^2(G_0 - 1)^2}{8Ma^2}, \quad (11)$$

where

$$G_0^2 = \frac{1}{2} + \frac{4Ma^2 U_0}{\hbar^2} + \left\{ \left(\frac{1}{2} + \frac{4Ma^2 U_0}{\hbar^2} \right)^2 + \left(\frac{4Ma^2 U_1}{\hbar^2} \right)^2 \right\}^{1/2}, \quad (12)$$

and two turning points as well as their properties are given by

$$y_A = \sinh(x_A/a) = \frac{-U_1 - \sqrt{U_1^2 - 4E_n(U_0 + E_n)}}{2E_n},$$

$$y_B = \sinh(x_B/a) = \frac{-U_1 + \sqrt{U_1^2 - 4E_n(U_0 + E_n)}}{2E_n}, \quad (13)$$

$$y_A + y_B = U_1/E_n, \quad y_A y_B = 1 + U_0/E_n.$$

The momentum $k(x)$ is

$$k(x) = \frac{\sqrt{-2ME_n}}{\hbar\sqrt{1+y^2}} \sqrt{(y_B - y)(y - y_A)}. \quad (14)$$

Now, let us calculate the first integral in eq. (7):

$$\begin{aligned} \int_{x_A}^{x_B} k(x) dx &= \int_{x_A}^{x_B} \frac{1}{\hbar} \sqrt{2M(E - V(x))} dx \\ &= \omega(E_n) \int_{y_A}^{y_B} \frac{\sqrt{(y_B - y)(y - y_A)}}{1 + y^2} dy \\ &= -\pi\omega(E_n) + \frac{a\pi\sqrt{M}}{\hbar} \sqrt{U_0 + \sqrt{U_0^2 + U_1^2}}, \end{aligned} \quad (15)$$

where $\omega(E_n) = a\sqrt{-2ME_n}/\hbar$. In the above calculation, the following integral formula [18] was used:

$$\begin{aligned} \int_a^b \frac{\sqrt{(b-y)(y-a)}}{1+y^2} dy &= \\ \frac{\pi}{2} \left\{ \sqrt{1+a^2} \sqrt{1+b^2} - ab + 1 \right\}^{1/2} - \pi. \end{aligned} \quad (16)$$

Now, by replacing E_n in eq. (15) by E_0 given in eq. (11), we obtain

$$\int_{x_{0A}}^{x_{0B}} k_0(x) dx = \frac{\pi}{2} \left[1 - G_0 + \frac{2a\sqrt{M}}{\hbar} \sqrt{U_0 + \sqrt{U_0^2 + U_1^2}} \right]. \quad (17)$$

Substituting eqs. (15) and (17) into eq. (7) leads to

$$-\pi \left[\frac{a\sqrt{-2EM}}{\hbar} - \frac{G_0 - 1}{2} \right] = n\pi. \quad (18)$$

From eq. (18) we get the eigenvalues

$$E_n = -\frac{\hbar^2(G_0 - 2n - 1)^2}{8Ma^2}, \quad (19)$$

where $n = 0, 1, 2, \dots, [(G_0 - 1)/2]$. This result is the same as that in [15].

Next we look at the asymmetric trigonometric Rosen-Morse potential

$$V(x) = U_0 \cot^2(\pi x/a) + U_1 \cot(\pi x/a), \quad (20)$$

where $U_0 > 0$, $x \in [0, a]$. We introduce a new variable $y = -\cot(\pi x/a)$, $y \in (-\infty, \infty)$. The turning points y_A and y_B are determined by solving $V(x) = E_n$, where

$$E_n = U_0 y^2 - U_1 y, \quad y_A + y_B = \frac{U_1}{U_0}, \quad y_A y_B = -\frac{E_n}{U_0}. \quad (21)$$

The momentum $k(x)$ between them is given by

$$k(x) = \frac{\sqrt{2\mu}}{\hbar} \sqrt{E_n - U_0 y^2 + U_1 y}, \quad (22)$$

$$k'(y) = -\frac{\sqrt{2\mu} U_0}{\hbar} \frac{y - U_1/(2U_0)}{\sqrt{E_n - U_0 y^2 + U_1 y}}.$$

Ma *et al.* found that the ground-state energy is

$$E_0 = \frac{\hbar^2 C^2}{2\mu} - U_0 - \frac{\mu U_1^2}{2\hbar^2 C^2}, \quad (23)$$

$$C = \frac{\pi}{2a} \left(1 + \sqrt{1 + \frac{8\mu a^2 U_0}{\pi^2 \hbar^2}} \right).$$

The integral of the momentum $k(x)$ is calculated as follows:

$$\begin{aligned} \int_{-x_B}^{x_B} k(x) dx &= \frac{\xi}{\pi} \int_{-y_B}^{y_B} \frac{\sqrt{(y_B - y)(y - y_A)}}{(y^2 + 1)} dy \\ &= -\xi + \frac{\xi}{\pi} \int_{-y_B}^{y_B} \frac{y(y_A + y_B) - y_A y_B + 1}{(1 + y^2) \sqrt{(y_B - y)(y - y_A)}} dy \\ &= -\xi + \frac{a\sqrt{2\mu}}{\hbar} \left| \text{Re} \left\{ \sqrt{E_n + U_0 - iU_1} \right\} \right|, \end{aligned} \quad (24)$$

where $\xi = a\sqrt{2\mu U_0}/\hbar$.

Now, by replacing E_n in eq. (24) with E_0 given in eq. (23), one has

$$\begin{aligned} \int_{x_{0A}}^{x_{0B}} k_0(x) dx &= -\xi + \frac{a\sqrt{2\mu}}{\hbar} \left| \text{Re} \left\{ \sqrt{E_0 + U_0 - iU_1} \right\} \right| \\ &= -\xi + aC. \end{aligned} \quad (25)$$

Substituting eqs. (24) and (25) into eq. (7) gives

$$\frac{a\sqrt{2\mu}}{\hbar} \left| \text{Re} \left\{ \sqrt{E_n + U_0 - iU_1} \right\} \right| = aC + n\pi, \quad (26)$$

from which we obtain the eigenvalues as

$$E_n = \frac{\hbar^2(aC + n\pi)^2}{2\mu a^2} - \frac{\mu a^2 U_1^2}{2\hbar^2(aC + n\pi)^2} - U_0, \quad (27)$$

where $n = 0, 1, 2, \dots$. When $U_1 = 0$, this result reduces to the symmetric case. This result is consistent with that in ref. [16].

Finally, let us consider the Manning-Rosen effective potential in D dimensions [19]. For this potential we introduce a new variable,

$$y = \frac{1}{e^{\alpha r} - 1}, \quad y'(r) = -\alpha y(1 + y). \quad (28)$$

Then the effective Manning-Rosen potential will be transformed to the form

$$\begin{aligned} V_{\text{eff.}}(r) &= \frac{\alpha^2}{q^2} \left\{ [\beta(\beta - 1) + \ell'(\ell' + 1)] y^2 \right. \\ &\quad \left. + [\ell'(\ell' + 1) - A] y \right\}, \quad \kappa^2 = \frac{2\mu}{\hbar^2}, \end{aligned} \quad (29)$$

where we used a suitable approximation $1/r^2 \simeq \alpha^2 e^{-\alpha r} / (1 - e^{-\alpha r})^2$.

We adopt the following notations for simplicity:

$$V_2 = \alpha^2 \delta / \kappa^2, \quad V_1 = \alpha^2 \gamma / \kappa^2, \quad V(r) = V_2 y^2 + V_1 y, \quad (30)$$

$$\delta = [\beta(\beta - 1) + \ell'(\ell' + 1)], \quad \gamma = [\ell'(\ell' + 1) - A].$$

Let y_A and y_B be two turning points satisfying $V(y_A) = V(y_B) = E_{n\ell}$. One finds

$$y_A + y_B = -\frac{V_1}{V_2}, \quad y_A y_B = -\frac{E_{n\ell}}{V_2}. \quad (31)$$

The momentum $k(r)$ is written as

$$\begin{aligned} k(y) &= \sqrt{2\mu V_2 (y - y_A)(y_B - y)} / \hbar, \\ k'(y) &= \frac{\sqrt{2\mu V_2}}{2\hbar} \left(\sqrt{\frac{y_B - y}{y - y_A}} - \sqrt{\frac{y - y_A}{y_B - y}} \right). \end{aligned} \quad (32)$$

Based on non-linear Riccati equation (1), one gets

$$\begin{aligned} \phi_0(y) &= m\alpha y + \frac{\alpha}{2} + \frac{\alpha\gamma}{2m}, \\ E_0 &= -\frac{\hbar^2 \alpha^2}{8\mu} \left(1 + \frac{\gamma}{m} \right)^2, \end{aligned} \quad (33)$$

where

$$m = \frac{1}{2} + \sqrt{\delta + \frac{1}{4}}, \quad \delta = m(m-1). \quad (34)$$

The integral of the momentum $k(r)$ is now calculated as

$$\begin{aligned} \int_{r_A}^{r_B} k(r) dr &= \int_{y_A}^{y_B} \frac{\sqrt{2\mu V_2(y-y_A)(y_B-y)}}{-\alpha\hbar y(1+y)} dy \\ &= -\pi\sqrt{\delta} \left(\sqrt{\frac{-V_1}{V_2} - \frac{E_{n\ell}}{V_2}} + 1 - \sqrt{\frac{-E_{n\ell}}{V_2}} - 1 \right). \end{aligned} \quad (35)$$

By using eq. (8) we have

$$\begin{aligned} &-\pi\sqrt{\delta} \left(\sqrt{\frac{-V_1}{V_2} - \frac{E_{n\ell}}{V_2}} + 1 - \sqrt{\frac{-E_{n\ell}}{V_2}} - 1 \right) \\ &+ \left[\pi\sqrt{\delta} \left(\sqrt{\frac{-V_1}{V_2} - \frac{E_0}{V_2}} + 1 - \sqrt{\frac{-E_0}{V_2}} - 1 \right) \right] = n\pi. \end{aligned} \quad (36)$$

One can thus immediately obtain the eigenvalues for the D -dimensional Manning-Rosen potential $E_{n\ell}$ as

$$E_{n\ell} = -\frac{\hbar^2\alpha^2}{8\mu} \left[\tau - \frac{A + \beta(\beta-1)}{\tau} \right]^2, \quad \tau = n + m, \quad (37)$$

where the relations $\delta - \gamma = A + \beta(\beta-1)$ and $\delta = m(m-1)$ are used.

In addition, this proper quantization rule applies to all exactly solvable potentials. The energy spectra of a solvable potential can be obtained easily by the method.

Concluding remarks. – As shown in the above discussions, the proper quantization rule (7) and (8) greatly simplifies the calculations of the complicated integrals in the previous works [4,5,12–17]. Before concluding this work, we summarize its advantages over the original quantization rule. First, in applying the original exact quantization rule, one must find the eigenvalue and eigenfunction of the ground state simultaneously to calculate the complicated quantum correction term, while with the proper quantization rule only the ground-state energy is sufficient to determine the energy levels of a quantum system. Second, by using the proper quantization rule we only need to calculate one of the two integrals. Finally, the most important point is that the expression of the proper quantization rule is more symmetrical than the original one. The beauty and simplicity of the rule come from its meaning — whenever the number of the nodes of $\phi(x)$ or the number of the nodes of the wave function $\psi(x)$ increases by one, the momentum integral $\int_{x_A}^{x_B} k(x) dx$ will increase by π .

We would like to thank the kind referee for positive and invaluable suggestions which improved the present manuscript greatly. One of the authors (S-HD) thanks Profs. ZHONG-QI MA and XIAO-YAN GU for helpful discussions and also Dr. BING He for reading carefully and improving the manuscript. This work is supported in part by Natural Science Basic Research Plan in the Shaanxi Province of China (program No. SJ08A13), the Natural Science Foundation of the Education Bureau of Shaanxi Province, China under Grant O9jk534 and partly by 20090513-SIP-IPN, COFAA-IPN, Mexico.

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