

## ENERGY SPECTRUM OF THE KRATZER INTERACTION

J.A.C. GALLAS

Max-Planck-Institut für Quantenoptik, Forschungsgelände, D-8046 Garching bei München, Federal Republic of Germany  
and Universidade Federal de Santa Catarina, Departamento de Física, 88000 Florianópolis, S.C., Brazil

Received 15 February 1983

Kesarwani and Varshni recently reported the WKB approximation to be capable of producing highly accurate eigenvalues for Kratzer's interaction, if an adequate number of *high-order* corrections were taken into account. We show that by making the Langer transformation, it is possible to reproduce the known exact results within the *first-order* theory.

Two recent papers in this journal discussed the energy spectrum of the Kratzer [1,2] interaction in semiclassical WKB approximation. The first of these [3] gave the impression that semiclassical eigenvalues are a poor approximation to the known exact eigenvalues. In the second of these Kesarwani and Vashni [4] pointed out that the above mentioned WKB results [3] were incorrect and that very high accuracy could be obtained if an adequate number of *high-order* terms were taken in the semiclassical approximation. In this note we show that the Langer-transformed *first-order* semiclassical quantization reproduces the known exact analytical results.

We start by introducing the interaction potential

$$V(r) = -2D(a/r - \frac{1}{2}q a^2/r^2), \quad (1)$$

where  $D > 0$  and  $a > 0$ . For later convenience we introduced in (1) a parameter  $q$  such that for  $q = 0$  eq. (1) reduces to a Coulomb potential while for  $q = 1$  the potential corresponds to Kratzer's interaction, whose spectrum is known [5] to be given by

$$E_{nl} = \frac{-D\gamma^2}{\{n + \frac{1}{2} + [\gamma^2 + (l + \frac{1}{2})^2]^{1/2}\}^2}, \quad (2)$$

where  $\gamma^2 = 2ma^2D/\hbar^2$ . The eigenfunctions for bound as well as for scattering states have been discussed by Flüge [5]. For completeness we also quote a paper by Stetter and Shatas [6] where some matrix elements for Kratzer's interaction were derived.

The radial equation describing the motion of a particle of mass  $m$  in a potential  $V(r)$  is given by

$$-(\hbar^2/2m)\psi'' + [V(r) + (\hbar^2/2m)L^2/r^2]\psi = E\psi, \quad (3)$$

where, as usual,  $L^2 = l(l+1)$ . The corresponding semiclassical approximation to the eigenvalues of (3) is obtained from

$$\int_{r_1}^{r_2} P(r) dr = (n + \frac{1}{2})\pi, \quad n = 0, 1, 2, \dots, \quad (4)$$

where

$$[P(r)]^2 = (2m/\hbar^2)[E - V(r) - (\hbar^2/2m)L^2/r^2], \quad (5)$$

and where now, owing to the Langer transformation [7],  $L^2 = (l + \frac{1}{2})^2$ . This transformation is connected with the boundary conditions obeyed by the eigenfunctions of radial equations [8]; it is known in the semiclassical treatment of, e.g. the hydrogenic spectrum [5,8,9] and the Stark effect [10]. Now, using the fact that

$$\int_{r_1}^{r_2} \frac{dr}{r} [-r^2 + (r_1 + r_2)r - r_1 r_2]^{1/2} = \frac{1}{2}\pi[r_1 + r_2 - 2(r_1 r_2)^{1/2}], \quad (6)$$

we identify

$$r_1 + r_2 = -2Da/E > 0, \quad (7a)$$

$$r_1 r_2 = -E^{-1} [Dqa^2 + (\hbar^2/2m)L^2] > 0, \quad (7b)$$

and obtain the semiclassical eigenenergies as

$$E_{nl}^{\text{WKB}} = \frac{-D\gamma^2}{[n + \frac{1}{2} + (q\gamma^2 + L^2)^{1/2}]^2}, \quad (8)$$

where  $L^2 = (l + \frac{1}{2})^2$ . For  $q = 0$  one obtains the hydrogenic spectrum as it should be. For Kratzer's interaction ( $q = 1$ ), eq. (8) reproduces the exact result (2).

The critical difference between the present calculation and the previously mentioned ones [3,4] is that they had  $L^2 = l(l + 1)$ . For the particular case discussed in [3,4], namely for  $s$  states, their formulas incorrectly give  $L^2 = 0$ . The numerics can easily be checked by taking  $D = 1$  and  $\gamma^2 = 50$ .

To conclude, it is tempting to conjecture that first-order calculations for a generalized form of (1) discussed in ref. [11] could also be improved by performing the Langer transformation.

The author is grateful to the Deutscher Akademischer Austauschdienst/Bonn for partial support.

## References

- [1] A. Kratzer, *Z. Physik* 3 (1920) 289; *Ann. Phys.* 67 (1922) 127.
- [2] E. Fues, *Ann. Phys.* 80 (1926) 367.
- [3] E. Yurtsever, O. Yilmaz and D.D. Shillady, *Chem. Phys. Letters* 85 (1982) 111.
- [4] R.N. Kesarwani and Y.P. Varshni, *Chem. Phys. Letters* 93 (1982) 545.
- [5] S. Flügge, *Practical quantum mechanics*, Vol. 1 (Springer, Berlin, 1971) problems 69, 116, 117, 120–123.
- [6] J.D. Stetter and R.A. Shatas, *Intern. J. Quantum Chem.* 5S (1971) 277.
- [7] R.E. Langer, *Phys. Rev.* 51 (1937) 669.
- [8] J.A.C. Gallas and R.F. O'Connell, *J. Phys.* B15 (1982) L593.
- [9] P.A. Vicharelli and C.B. Collins, *Phys. Letters* 89A (1982) 215.
- [10] J.A.C. Gallas, H. Walther and E. Werner, *Phys. Rev. Letters* 49 (1982) 867.
- [11] R.N. Kesarwani and Y.P. Varshni, *Can. J. Phys.* 56 (1978) 1488; 58 (1980) 363.