

ENERGY SPECTRUM OF THE KRATZER INTERACTION

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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.

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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.