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Comment on "Breakdown of Bohr's correpondence principle"

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Abstract

It is shown that the statement madeby Bo Gao in Phys. Rev. Lett. **83** 4225 (1999) regarding the breakdown of Bohr's correspondence principle for singular potentials is incorrect; it originates in a misinterpretation of the quasi-classical approximation, and the disregard of the short-range cut-off for such potentials.

In a recent letter[1] Bo Gao claims that the quasi-classical approximation and Bohr's correspondence principle break down for potentials having an attractive tail of the form $-C_n/r^n$ for $r \to \infty$ and $n > 2$. This is an incorrect assertion, originating in a misinterpretation of Bohr-Sommerfeld's quantization rules, the overlooking of the finite threshold energy for the bound states, and the "fall-on-the-centre" phenomenon (for $r \to 0$) specific to such singular potentials.

Bohr-Sommerfeld's quasi-classical quantization rules read

$$\oint p_r dr = \oint \left[2\mu(-|E| - U_l)\right]^{1/2} dr = 2\pi\hbar(v + 1/2) \quad , \tag{1}$$

for the radial motion of a particle of mass μ in a central attractive potential $V(r)$, where

$$U_l = V(r) + \hbar^2 l(l+1)/2\mu r^2 \tag{2}$$

includes the centrifugal repulsion, and v denotes an integral (quantum) number. Equation (1) is valid for large values of the classical action as compared with Planck's constant $\hbar$, *i.e.* for large values of the quantum number v, and, consequently, for a large number of energy levels labelled by v; it implies the geometrical-optics condition $|d\lambda/dr| \ll 1$ ($\lambda = 2\pi\hbar/p_r$) be satisfied over as large parts of the classical trajectory as possible, as well as the energy quanta $\Delta|E| = \hbar\omega$, where ω is the classical frequency, be much smaller than the the kinetic energy $E_r = p_r^2/2\mu$. The geometrical-optics condition can also be written as

$$\pi\hbar \left|dU_l/dr\right| \ll p_r E_r \quad , \tag{3}$$

and it is violated near the turning points of the trajectory; however, within the quasi-classical approximation, the region where this condition breaks down is much smaller than the rest of the trajectory.[2]

Indeed, the bound-states spectrum of potentials behaving at infinite like $-C_n/r^n$ where $n > 2$ has a threshold of finite, non-vanishing energy $-|E_0|$ (in contrast with the Coulomb potential); this

point is overlooked in Ref.1, in assessing the validity of the quasi-classical approximation; for any fixed l and a sufficiently large value of C_n the classical trajectory corresponding to this threshold energy has an outer turning point located at $r_t \sim (C_n/|E_0|)^{1/n}$, as for the s-states analyzed in Ref.1. An expansion around this turning point shows that the condition (3) is violated over a distance $|r - r_t|$, such that

$$|r - r_t| / r_t \sim (\pi^2 \hbar^2 / 2\mu n)^{1/3} C_n^{-2/3n} |E_0|^{(2-n)/3n} \quad ; \tag{4}$$

one can see that $|r - r_t| / r_t \ll 1$ for any finite value of E_0 providing C_n is sufficiently large; therefore the quasi-classical approximation holds for the top of the spectrum, in contrast with the claim made in Ref.1. For large values of C_n, and of the efective potential U_l, an expansion of (1) in powers of $|E|$ leads to

$$|E| = A_l(v_{\max} - v + B_l) \tag{5}$$

for the energy levels at the top of the spectrum (within the linear approximation), where

$$\begin{aligned} A_l^{-1} &= (4\pi\hbar)^{-1} \oint (-U_l/2\mu)^{-1/2} dr \quad , \\ B_l &= (2\pi\hbar)^{-1} \oint (-2\mu U_l)^{1/2} dr - 1/2 - v_{\max} \quad , \end{aligned} \tag{6}$$

and $v_{\max}$ is the maximum value of the quantum number, corresponding to the threshold energy $|E_{0l}| = A_l B_l$; one can see that B_l (which can be related to the number of levels) has large values, and the level inter-spacing A_l is small in comparison with the average kinetic energy; this inter-spacing is not a "universal" constant as claimed in Ref.1, but depends on the behaviour of the effective potential U_l over its entire range ($U_l < 0$), including its short-range behaviour. This type of formulae had to be employed in Ref.1 in order to compare the quasi-classical approximation with quantum-mechanical calculations.

If the potential $-C_n/r^n$ with $n > 2$ is extended to $r \to 0$ then the spectrum is not bounded from below and the particle "falls on the centre"; a large cut-off is then necessary to be imposed upon the potential, located at very short distances. The condition (3) is satisfied for $r \to 0$, so that the quasi-classical approximation may be extended to lower-energy levels, corresponding to states which are highly localized at the origin; the integral in (1) can now be estimated easily, as the main contribution to it comes from the small region around the origin; within the first approximation the integration may be limited to $r_t \simeq (C_n/|E|)^{1/n}$, but higher-order corrections are necessary for more accurate estimations; with the customary energy scale $E = \alpha_n (\hbar^2/2\mu)^{n/(n-2)} C_n^{2/(2-n)} \varepsilon$, where α_n is a numerical parameter, one obtains

$$|\varepsilon|^{(n-2)/2n} = A_n \left[1 - (n-2)A_n/4n + ...\right] (v_{\max} - v + \mu_D) \quad , \tag{7}$$

where

$$A_n = \frac{1}{2} \pi (n-2) \alpha_n^{(2-n)/2n} \tag{8}$$

and μ_D is a constant associated with the maximum value $v_{\max}$ of the quantum number, and originating in the short-range cut-off imposed upon the potential for $r \to 0$. For $n = 3$ and $\alpha_n = 4$, as in Ref.1, one obtains $|\varepsilon|^{1/6} = 1.11(v_{\max} - v + \mu_D)$, which is the formula[3] employed in Ref.1; for $n = 6$ and $\alpha_n = 16$ one gets $|\varepsilon|^{1/6} \simeq 1.45(v_{\max} - v + \mu_D)$, and higher-order corrections are necessary to (7) in order to get a more accurate value for the numerical coefficient (1.93 according to Ref. 3 and Ref.1); in agreement with Ref.1 (for s-states and $n = 3$ and $n = 6$), the quasi-classical approximation of the type given by (7), and Bohr's correspondence principle are validated by quantum-mechanical calculations for lower-energy levels, as expected; and the

level inter-spacing is indeed a "universal" constant now ($\Delta(\varepsilon^{1/6}) = 1.11$, for instance, for $n = 3$); these levels corresponds to high quantum numbers $v_{\max}$, as compared with the "bottom" of the potential, and one can see that the short-range behaviour of the potential, and the corresponding cut-off, are essential for a consistent picture. However, the formula (7) is not applicable for the top of the spectrum, as misinterpreted in Ref.1; instead, formulae of the type given by (5) are appropriate in this case, with a proper short-range cut-off for the singular potential.

Finally, one may say that quasi-classical approximation and Bohr's correspondence principle hold, even for singular potentials of the form $-C_n/r^n$ where $n > 2$, which exibit the "fall-on-the-centre" phenomenon; however, these potentials are unphysical, and the realistic potentials which correspond to the photoassociative atomic spectroscopy exhibit a highly repulsive short-range part; in this case the quasi-classical approximation is described by formulae of the type given by (5) for the top of the spectrum.

References

[1] Bo Gao, Phys. Rev. Lett. **83** 4225 (1999).

[2] See, for instance, R. E. Langer, Phys. Rev. **51** 669 (1937), and Phys. Rev. **75** 1573 (1949).

[3] R. J. LeRoy and R. B. Bernstein, J. Chem. Phys. **52** 3869 (1970).