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Comment on "Breakdown of Bohr's correpondence principle"

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Abstract

It is shown that the statement made by Bo Gao in Phys. Rev. Lett. **83** 4225 (1999) regarding Bohr's correspondence principle is incorrect; it originates in misapplication of the quasi-classical approximation, and the disregard of the short-range cut-off for singular 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 $n > 2$. The purpose of this comment is to show this assertion is incorrect. In his argumentation the author of Ref.1 resorts to both his published[2] and unpublished quantum-mechanical calculations, as well as to extrapolations of such calculations; however, he overlooks the finite threshold energy for the bound states, and misinterprets the energy spectrum as derived from Bohr-Sommerfeld's quantization rules for such potentials; in addition, he overlooks the "fall-on-the-centre" phenomenon, specific to potentials behaving like $-1/r^n$ for $r \to 0$ and $n > 2$.

With usual notations the radial Schrodinger equation reads

$$(p_r^2/2\mu + U_l)\psi = E\psi \quad , \quad U_l = V(r) + \hbar^2 l(l+1)/2\mu r^2 \quad , \tag{1}$$

where p_r is the radial momentum and $V(r)$ is a central potential; according to the quasi-classical approximation

$$p_r = [2\mu(-|E| - U_l)]^{1/2} \quad , \tag{2}$$

and Bohr-Sommerfeld's quantization reads

$$\oint p_r dr = 2\pi\hbar(v + 1/2) \quad , \tag{3}$$

where v is an integral (quantum) number; the integration in (3) is performed over the entire classical orbit, as for quantum bound states in an attractive potential $V(r)$; for large values of l the quasi-classical expression $(l + 1/2)^2$ must be substituted for the quantum value $l(l + 1)$ of the square angular momentum. The approximation is valid for values of the classical action much larger than Planck's constant $\hbar$, *i.e.* for large quantum numbers v, and, therefore, for a large number of energy levels labelled by v; this implies the spatial variation of the wavelength $\lambda = 2\pi\hbar/p_r$ be as small,

$$|d\lambda/dr| \ll 1 \quad , \tag{4}$$

over as large part of the orbit as possible (like in the geometrical optics), and the inter-spacing $\Delta E = \hbar\omega$ of the energy levels (*i.e.* quanta of energy), where ω is the classical frequency, be much smaller than the kinetic energy $E_r = p_r^2/2\mu$; this is the content of the quasi-classical approximation and Bohr's correspondence principle. The condition (4) of geometrical optics can also be written as

$$\pi\hbar \left| dU_l/dr \right| \ll p_r E_r \quad , \tag{5}$$

and it is not satisfied near the turning points of the trajectory, where $p_r \to 0$; however, if for the rest of the trajectory the kinetic energy is sufficiently high, which implies high values of $-U_l$, the condition is fulfilled, and the quasi-classical approximation (and Bohr's correspondence principle) are valid; on the contrary, if the condition (4) is violated over a large part of the trajectory, then the quasi-classical approximation and Bohr's corerspondence principle break down. Within the classical approximation the extent of the region close to the turning points is small in comparison with the rest of the trajectory.[3]

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 $-\left|E_0\right|$ (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 $r_t \sim (C_n/\left|E_0\right|)^{1/n}$, as for the s-states analyzed in Ref.1. An expansion around this turning point shows that the condition (5) is violated over a distance $|r - r_t|$, such that

$$\left|r - r_t\right| / r_t \sim (\pi^2\hbar^2/2\mu n)^{1/3} C_n^{-2/3n} \left|E_0\right|^{(2-n)/3n} \quad ; \tag{6}$$

one can see that $\left|r - r_t\right| / r_t \ll 1$ 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.

The value of the threshold energy $\left|E_0\right|$ is determined by the behaviour of the potential U_l over short distances; it may be characterized by an average value U_{l0} over a distance scale R_l; for a quasi-classical spectrum $-U_{l0}$ must be large (in accordance with the large values of C_n), and the threshold energy $\left|E_0\right|$ has a small, but non-vanishing, value. Making use of the parameters U_{l0} and R_l one may estimate the quasi-classical spectrum near the threshold $-\left|E_{l0}\right|$; indeed, since $|E|$ is small at the top of the spectrum, one may expand (3) in powers of $|E|$; within the linear approximation one obtains

$$|E| = 2(-U_{l0}) - 2\pi\hbar(-U_{l0}/2\mu R_l^2)^{1/2}(v + 1/2) \quad , \tag{7}$$

or

$$|E| = |E_{l0}| + 2\pi\hbar(-U_{l0}/2\mu R_l^2)^{1/2}(v_{\max} - v) \quad , \tag{8}$$

where the maximum quantum number $v_{\max}$ corresponds to the threshold energy; one can see that the spectrum is linear (for small values of $v_{\max} - v$) to the first approximation, and the level inter-spacing $\Delta\left|E\right| = 2\pi\hbar(-U_{l0}/2\mu R_l^2)^{1/2}$ is not a "universal" constant as claimed in Ref.1, but it depends on the short-range specific form of the potential (it has also a slight dependence on l). In addition, $\Delta\left|E\right| / E_r \sim \hbar(-2\mu U_{l0} R_l^2)^{-1/2} \ll 1$ for large values of the classical action $(-2\mu U_{l0} R_l^2)^{1/2}$, so that Bohr's correspondence principle is valid. It is also worth noting that the total number of levels N_l within the quasi-classical approximation is given by

$$N_l = \int dp_r dr/(2\pi\hbar) = \frac{(2\mu)^{1/2}}{2\pi\hbar} \oint (-U_l)^{1/2} dr \quad , \tag{9}$$

and making use of the parameters introduced above one obtains $N_l = (-2\mu U_{l0})^{1/2} R_l/\pi\hbar$; hence, the energy levels (7) may also be written as

$$|E| = 2(-U_{l0})\,[1 - (v + 1/2)/N_l] \quad , \tag{10}$$

and the threshold energy becomes

$$|E_{l0}| = 2(-U_{l0})\,[1 - (v_{\max} + 1/2)/N_l] \quad ; \tag{11}$$

one can see that, since $v_{\max}/N_l$ is slightly less than unity (for large $v_{\max}$ and N_l), the threshold energy has indeed a small, but non-vanishing, value. For a comparison with quantum-mechanical calculations, as attempted in Ref. 1, formulae of the type (7) and (8) should be employed for the top of the spectrum (higher-order corrections included), and they depend non-trivially on the details of the shorter-range part of the potential.

If the potential $-C_n/r^n$ where $n > 2$ is extended towards $r \to 0$ 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 (5) is satisfied for $r \to 0$, so that the quasi-classical approximation may be extended to lower-energy levels, corresponding to states highly localized at the origin; the integral in (3) 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 $r_t \simeq (C_n/\,|E|)^{1/n}$, leading to

$$|E|^{(n-2)/2n} = \frac{\pi\hbar(n-2)}{2(2\mu)^{1/2}} C_n^{-1/n} (v_{\max} - v + const) \quad , \tag{12}$$

where a constant *const* is associated with the maximum value of the quantum number; it originates in the short-range cut-off imposed upon the potential for $r \to 0$; it is customary to scale the energy as $E = \alpha_n (\hbar^2/2\mu)^{n/(n-2)} C_n^{2/(2-n)} \varepsilon$, where α_n are numerical parameters, so that (12) becomes

$$|\varepsilon|^{(n-2)/2n} = A_n (v_{\max} - v + \mu_D) \quad , \tag{13}$$

where μ_D is another customary notation used in Ref.1, corresponding to the constant in (12), and

$$A_n = \frac{1}{2}\pi(n-2)\alpha_n^{(2-n)/2n} \quad ; \tag{14}$$

the next-order correction to (13) gives an additional prefactor $1 - (n-2)A_n/4n$ so that one gets

$$|\varepsilon|^{(n-2)/2n} = A_n\,[1 - (n-2)A_n/4n + ...]\,(v_{\max} - v + \mu_D) \quad ; \tag{15}$$

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 (15) 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 $n = 3$ and $n = 6$), the quasi-classical approximation of the type given by (15), 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 (15) is not applicable for the top of the spectrum, as misinterpreted in Ref.1; instead, formulae of the type given by (7) and (8)

are appropriate in this case (higher-order corrections included), 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 (7) and (8) for the top of the spectrum.

References

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

[2] Bo Gao, Phys. Rev. **A58** 1728, 4222 (1998); Phys. Rev. **A59** 2778 (1999).

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

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