Comment on "Breakdown of Bohr's Correspondence Principle"

In Ref. [1], it is shown that the Bohr's Correspondence Principle (BCP) breaks down "in all quantum systems in which the asymptotic interaction between the fragments behaves as $-C_n/r^n$ with $n > 2$." We show here that this failure is due to the use of a not rigorous form of BCP, and we give a correct form of BCP.

BCP is defined in Ref. [1] as "the expectation that the semiclassical approximation works better for states with greater quantum numbers." This form is easily violated, for instance, by an anharmonic 1D oscillator. The semiclassical quantization condition is excellent for the low lying levels, if the potential is accurately harmonic, and will be less accurate for some higher levels, if the semiclassical validity condition is locally violated for these levels.

A strict form of BCP should involve the comparison of classical and quantum dynamics at a fixed energy E, in the limit $\hbar \to 0$. Because it is difficult to apply the semiclassical approximation for nonseparable problems in larger dimensions, we consider only 1D problems. A time-independent form of BCP is the following: if $a(r)$ is any smooth function of r, for a given energy E, the quantum and classical averages of this function tend toward the same limit when $\hbar \to 0$. The classical average is the time weighted average

$$\langle a \rangle_{\rm cl} = \oint a(r)\, dt \Big/ \oint dt\,,$$

with $dt = dr/v(r)$, where $v(r)$ is the velocity. The quantum average is

$$\langle a \rangle_q = \int a(r)\, |\Psi(r)|^2\, dr \Bigg/ \int |\Psi(r)|^2\, dr\,,$$

where $\Psi(r)$ is the wave function. The quantum average is always defined in the continuum. In the region of bound levels, it is defined only when $\hbar$ is such that E is the energy of a bound level. If the JWKB approximation applies everywhere, the two averages are easily shown to be equal when $\hbar \to 0$.

In the case of an interaction of the form $-C_n/r^n$ with $n > 2$, the JWKB approximation fails near the dissociation energy $E = 0$. In the continuum ($E > 0$), this is the quantum threshold regime described by Wigner [2]. Following Julienne and Mies [3], this regime extends over an energy range extending from $E = 0$ up to the quantum threshold energy E_Q. E_Q scales like $\hbar^\gamma$ with the exponent $\gamma = 2n/(n-2)$ larger than 2. For bound states, a similar problem arises, described first by Le Roy and co-workers [4] and also by [5,6]. This is the mirror image for bound states of the quantum threshold regime in the continuum [7] extending over a comparable energy range. For any fixed energy $E \neq 0$, when $\hbar$ is sufficiently small, $E_Q < |E|$ and our formulation of BCP will be valid.

The case $E = 0$ requires a special discussion. At large r, the classical weight is given by $1/v(r) \propto r^{n/2}$, while the quantum weight is the square of the zero energy wave function with an asymptotic behavior given by $\Psi(r) \propto (cr + d)$ where c and d are constant. These two weights are different and, at first sight, the resulting averages should be different, but as the integral of these two weights are both divergent when $r \to \infty$, the two averages are of limited interest: for instance, they vanish for any function $a(r)$ which differs from zero only in a finite r range. The $E = 0$ case is a limiting case between finite and infinite classical trajectories, between discrete levels and continuum in quantum mechanics, and this character explains an apparent failure of BCP in this case.

Finally, the important point is the existence of two noncommuting limits in the mathematical sense ($E \to 0$ and $\hbar \to 0$) and the form of BCP used by Gao [1] consists precisely in letting the energy go close to zero at a fixed $\hbar$ value. The rigorous time-independent form of BCP proposed here is valid everywhere except for zero energy. Finally, the analytical results obtained by Gao will surely help and complement our understanding of the highest vibrational levels which are highly nonclassical, as shown by previous works [4–7].

C. Boisseau,[1,*] E. Audouard,[2] and J. Vigué[1]
[1]Laboratoire Collisions Agrégats Réactivité
Université Paul Sabatier
CNRS UMR 5589
118, Route de Narbonne
31062, Toulouse Cedex, France
[2]Laboratoire Traitement du Signal et Instrumentation
Université Jean Monnet
CNRS UMR 5516
23, rue du docteur Paul Michelon
42023, Saint-Etienne Cedex 2, France

Received 28 February 2000
DOI: 10.1103/PhysRevLett.86.2694
PACS numbers: 03.65.–w, 31.15.Gy, 33.20.Tp

*Present address: Department of Physics, University of Connecticut, 2152 Hillside Road U-46, Storrs, Connecticut, 06269.
Email address: boisseau@phys.uconn.edu

[1] B. Gao, Phys. Rev. Lett. **83**, 4225 (1999).
[2] E. P. Wigner, Phys. Rev. **73**, 1002 (1948).
[3] P. S. Julienne and F. H. Mies, J. Opt. Soc. Am. B **6**, 2257 (1989).
[4] S. M. Kirschner and R. J. Le Roy, J. Chem. Phys. **68**, 3139 (1979); R. Paulson, F. Karlsson, and R. J. LeRoy, J. Chem. Phys. **79**, 4346 (1983).
[5] J. Trost, C. Eltschka, and H. Friedrich, J. Phys. B **31**, 361 (1998); J. Trost, C. Eltschka, and H. Friedrich, Europhys. Lett. **43**, 230 (1998).
[6] C. Boisseau, E. Audouard, and J. Vigué, Europhys. Lett. **41**, 349 (1998).
[7] C. Boisseau, E. Audouard, J. Vigué, and V. V. Flambaum, Eur. Phys. J. D **12**, 199 (2000); C. Boisseau, thesis, University Paul Sabatier, 1999.

 0031-9007/01/86(12)/2694(1)$15.00