Nuclear Physics Approach

COMMENT ON EXACT UPPER BOUND ON BARRIER PENETRATION PROBABILITIES IN MANY-BODY SYSTEMS

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Abstract

We investigate conditions under which it is not possible to establish an exact upper bound for the barrier penetration probability of nuclei tunneling to classically forbidden small relative separation, by a value calculable in terms of the Born–Oppenheimer potential between nuclei.

1. Introduction

Leggett and Baym (LB) [1] investigated an upper bound on barrier penetration probabilities in many–body systems and claimed to obtain the result that the rate of tunneling of nuclei to classically forbidden small relative separation, in a fully interacting quantum–mechanical many–body system in equilibrium, is rigorously bounded above by a value calculable in terms of the Born–Oppenheimer potential between the nuclei. As LB cautioned in their paper, this potential can differ from conventional Born-Oppenheimer potential. In this report, we describe the conditions under which it is not possible to obtain such an exact upper bound.

2. Outline of the Derivation by LB

LB [1] start from a stationary–state wave function $\psi(\vec{r},\vec{\xi})$ of the many–body system,

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + \widehat{H}(r)\right]\psi(\vec{r},\vec{\xi}) = E\psi(\vec{r},\vec{\xi}) \ , \tag{1}$$

and obtain

$$\int d\xi \psi^*(\vec{r},\vec{\xi})\widehat{H}(r)\psi(\vec{r},\vec{\xi}) \geq U(\vec{r})\rho(\vec{r}) \ , \tag{2}$$

where

$$\rho(\vec{r}) = \int d\xi |\psi(\vec{r},\vec{\xi})|^2 \ , \tag{3}$$

$\vec{r}$ is the relative deuteron pair coordinate and $\vec{\xi}$ are all other coordinates. Using eqs. (1) and (2), and the Schwartz inequality, they obtain

$$\frac{\hbar^2}{2\mu}\frac{\Delta\chi(\vec{r})}{\chi(\vec{r})} \geq U(\vec{r}) - E \ , \tag{4}$$

where

$$\chi(\vec{r}) \equiv \rho(\vec{r})^{1/2} \ . \tag{5}$$

They introduce a potential $V_1(\vec{r})$, defined as

$$V_1(\vec{r}) \equiv \frac{\hbar^2}{2\mu}[\Delta\chi(\vec{r})]/\chi(\vec{r}) + E \ , \tag{6}$$

and, using eqs. (4) and (6), write the following bounds

$$V_1(\vec{r}) \geq U(\vec{r}) \geq V_2(\vec{r}) \ , \tag{7}$$

where $U(\vec{r})$ is the effective potential in the Born–Oppenheimer approximation, and $V_2(r)$ is a direction–independent lower bound on $U(\vec{r})$. From eq. (7), they find that the Born–Oppenheimer approximation leads to an upper bound on the barrier penetration probability.

3. Validity of the Exact Upper Bound by LB

We first note that Eq.(2) is valid for the wave function, which is normalizable over $\vec{\xi}$. For the initial state of $d+$ metal, for which d is free in the continuum, we do not expect $\int d\vec{\xi}|\psi(\vec{r},\vec{\xi})|^2 < \infty$, because the $d+$ metal system is multichannel system. Therefore, Eq.(7) is valid only for the case in which all particles form a bound state.

Introducing $\phi(r)$ as the regular s-wave solution of the Schroedinger equation

$$-\frac{\hbar^2}{2\mu}\Delta\phi + V_2\phi = E\phi, \tag{8}$$

it is straightforward to obtain, for any $r \leq r_0(E)$, ($r_0(E)$ is the largest distance for which $V_2(r) - E \geq 0$), a general inequality given by Eq.(1) of LB [1]:

$$\ell n\left[\frac{\rho(r)}{\rho(0)}\right] \geq \ell n\left[\frac{\phi^2(r)}{\phi^2(0)}\right]. \tag{9}$$

Noting that $\phi^2(r) \geq \phi^2(0)$ for $r \leq r_o(E)$, we can obtain from Eq.(9) the following inequality,

$$\rho(0) \leq \int_0^{r_0(E)} \rho(r)r^2dr \cdot \phi^2(0)[\int_0^{r_0(E)} \phi^2(r)r^2dr]^{-1}. \tag{10}$$

If we assume as in ref. [1] that $\int_0^{r_o(E)} \rho(r)r^2dr = \frac{1}{4\pi}$, and $\phi(r) = F_0(r)/r$, where $F_0(r)$ is the regular Coulomb wave function with screening energy for $(d+d)$, then we obtain the inequalaity given in Eq.(10) of ref. [1].

We note that LB [1] use the following definition of reaction rate R

$$R = A\rho(0) \tag{11}$$

where A is the nuclear constant. Eq.(11) is not valid since the nuclear interaction range is not equal to zero. In general, the reaction rate from the ℓ-partial wave contribution, R_ℓ, can be written as [2]

$$R_\ell \propto \int_0^\infty \rho_\ell^{1/2}(r) U_\ell(r, r') \rho_\ell^{1/2}(r') r^2 dr r'^2 dr', \tag{12}$$

where $U_\ell(r, r') = Im < r|T_\ell|r' >$ with T representing the ℓ-th partial wave contribution of the elastic T-matrix operator. It is shown [2] that, if $U_\ell(r, r')$ has a weak component with a finite long-range interaction, the upper bound given by LB [1] is not valid.

4. Conclusions

The exact upper bound given by LB [1] is not valid,
(i) if many-body system (electrons, nuclei) does not form a stationary bound state, and also
(ii) if the imaginary part of the effective nuclear interaction in the elastic channel has a very weak component with a finite long interaction-range.

References

[1] A.J. Leggett and G. Baym, Phys. Rev. Lett. **63**, 191 (1989).
[2] Y.E. Kim and A.L. Zubarev, Nuov. Cim. **108A**, 1009 (1995).