THE CLASSICAL SCHRÖDINGER EQUATION AS FIELD THEORY IN COMPLEX SPACE

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Abstract

The Classical Schrödinger Equation (CSE), i.e. the Schrödinger equation where the Hamiltonian has Bohm's quantum potential substracted,

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m}\nabla^2+V(x,t)+\frac{\hbar^2}{4m}\left(\frac{\psi^*(x,t)\psi(x,t)\nabla^2\left(\psi^*(x,t)\psi(x,t)\right)-\frac{1}{2}\left[\nabla\left(\psi^*(x,t)\psi(x,t)\right)\right]^2}{\left(\psi^*(x,t)\psi(x,t)\right)^2}\right)\right\}\psi(x,t)$$

(1)

is shown to arise from a complex field, built up from the real fields $R(x,t)$ and $S(x,t)$, with $\psi(x,t)=R(x,t)e^{\frac{i}{\hbar}S(x,t)}$ and $\psi^*(x,t)=R(x,t)e^{-\frac{i}{\hbar}S(x,t)}$, if one starts from the classical Hamilton–Jacobi and continuity equations for $R(x,t)$ and $S(x,t)$ and then uses a suitable variational procedure[1]. Equation (1) may also be termed the classical statistical mechanics equation for an ensemble of non–interacting particles described by the fields $R(x,t)$ and $S(x,t)$.

It is not difficult to show that CSE admits a reformulation in terms of a classical Green's function (where it is shown to depend on the wavefunction itself) and, ultimately, a classical Heisenberg matrix cast. Therefore, solution algorithms may be applied within the realm of quantum language, as already pointed out by Rosen some decades ago[2]. A practical solution to equation (1) has thus been implemented, by means of a Self–Consistent numerical procedure, based in turn on a Dirac–Frenkel variational principle and a discrete variable representation for the energy matrix.

Numerical results for benchmark systems show promising. In particular, the deep tunneling regime in Eckart barrier transmission is fairly close to the accurate quantum value, so that it considerably improves previous estimates by other semiclassical methods. Algebraic aspects, convergence issues (including quantum potential singularities), approximate treatments, extension to higher dimensionalities, as well as physical insight, have also been analyzed and will be presented in detail at the Workshop.

[1] A.S. Sanz, X. Giménez, J.M. Bofill and S. Miret–Artés, Chem. Phys. Lett. 478 (2009) 89; 488 (2010) 235 (erratum).
[2] N. Rosen, Am. J. Phys. 32 (1964) 597.