B.3. Phase-Amplitude Method-- *E.Y. Sidky and I. Ben-Itzhak*

Frequently in physics one-dimensional potentials are employed to model quantum systems, for example, alpha decay, nano-structures, field ionization or molecular ion dissociation. Even such simplified models can be difficult to solve if the potential is complicated, the reduced mass is large or tunneling is important. Thus, one often resorts to the semi-classical approximation [1,2]. For finding energy levels of one-dimensional potentials such an approximation is adequate; however, if one is interested in the lifetime of metastable states, which decay through tunneling, semi-classical theory can be very inaccurate. Numerically exact treatments are available [3-5]; however, these methods are not easy to apply mainly because of the time consuming search for narrow resonances coupled with the difficulty to define automatic criteria for such searches. Moreover, most methods rely on direct integration of the Schrödinger equation, which is numerically challenging when many nodes in the wave function are present or there is a strong exponential growth caused by large potential barriers. Responding to the need for an accurate, easy to use replacement for the commonly used semi-classical program [6], we have developed a general utility program (available upon request) based on improvements [Publication #81] to the Milne phase-amplitude method [7]. We also have applied it in the area of molecular ion physics [8] [Publication #86] and field ionization [10].

The wave function for the Milne method [7] is expressed in terms of two real variables

$$\psi = \sqrt{\tfrac{\pi}{2\mu}}\,\alpha(r)\sin(\phi(r));$$

α is the amplitude, and ϕ is the phase of the wave function. Substituting ψ into the wave equation leads to two coupled non-linear equations for α and ϕ

$$\frac{d^2\alpha}{dr^2} + k^2(r)\alpha = \frac{1}{\alpha^3}$$

$$\frac{d\phi}{dr} = \frac{1}{\alpha^2},$$

where $k^2(r) = 2\mu(E - V(r))$. E is the energy; $V(r)$ is the potential and μ is the reduced mass.

The phase-amplitude parameterization is related to semi-classical theory, which is obtained simply by setting $d^2\alpha/dr^2$ to zero, and as such it lends itself well to numerical solution of the Schrödinger equation since α and ϕ are smooth functions. The Milne method, however, does not treat potential barriers effectively. The amplitude diverges exponentially in classically forbidden regions, and it will oscillate wildly upon traversing a barrier.

We have made the following improvements to the Milne theory [7] in order to extend its applicability to any one-dimensional system [Publication #81]:

1. Replaced amplitude α with the log-amplitude $\gamma=\ln(\alpha)$. Solving for the log-amplitude allows for accurate evaluation of the wave function in classically forbidden regions, since it does not diverge rapidly.

2. Developed automatic scheme to divide potential into sections in which phase-amplitude parameters vary smoothly. This is necessary to build a solution valid over the whole domain of the system with a minimum of numerical effort.

3. Showed how the phase dependence on energy can be used to find resonances and their widths. Figure 1 shows how the Milne phase varies with energy for the metastable electronic ground state of $^{3}\mathrm{He}^{4}\mathrm{He}^{2+}$. Results are obtained from the He_2^{2+} potential energy curve computed by Ackermann and Hogreve [9]. Four vibrational resonances are found and their mean lifetimes range from 378 s for $\nu=0$ to 2.6 ps for $\nu=3$.

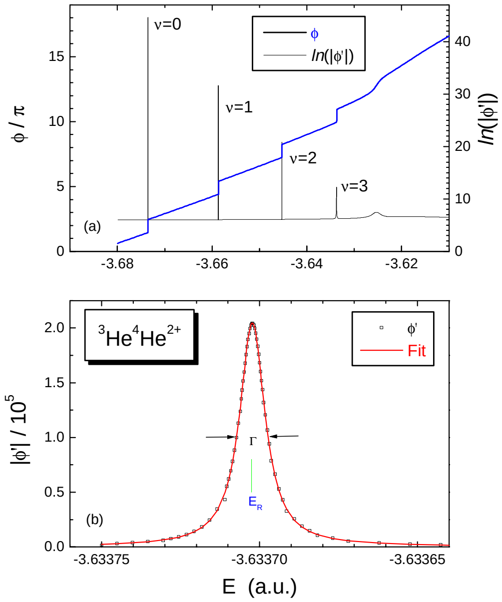

Figure 1. The resonances of $^{3}\mathrm{He}^{4}\mathrm{He}^{2+}$ found by the Phase-Amplitude method. **Top panel**: The phase and the natural logarithm of its derivative as a function of energy. Resonances are associated with a shift of π in the former and a peak in the latter. **Bottom panel**: The shape of the ϕ' peak for the $\nu=3$ resonance. A Lorentzian + constant fit the peak nicely.

In addition to the article describing the extensions to the Milne method [Publication #81], we have created a versatile utility program for analyzing one-dimensional problems. As input one simply gives the reduced mass of the system, the energy at which a wave function calculation is desired, the energy range over which one wants a scan for resonances and bound states, and the potential in numerical and/or analytic form. As output one gets bound state energies, resonance energies and widths, and the corresponding wave functions. It is important to note that continuum wave functions can be evaluated as easily and one can compute overlap integrals for bound free transitions. The program has already been employed for a variety of purposes: finding resonances in the CH^{2+} system, which is expected to decay by tunneling if it has metastable states [Publication #86]; calculating wave functions needed to evaluate the predissociation lifetimes for some states of CO^{2+} [8]; computing tunneling rates of all He_2^{2+} isotopes for future experiments (see proposal A.3.7); and computing field ionization rates of a model H_2^+. Furthermore, the simplicity of the method and program makes it a nice tool for teaching quantum mechanics and numerical methods at the graduate and undergraduate level, as we have done recently.

References

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