A Spatial Finite Size Scaling Method for calculation of Critical Parameters for Weakly Bound States

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Abstract

We present a finite size scaling approach to calculate critical parameters and exponents of quantum few-body system for which a bound state energy becomes absorbed or degenerates with the continuum. The scaling is done by introducing a cutoff radius for the potential. The asymptotic behavior for large values of the cutoff parameter is determined by the exact critical parameters.

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Weakly bound states represent an interesting field of research in atomic and molecular physics. The study of threshold effects in quantum few-body systems is motivated by the recent intense activity related with collision processes[1], quantum halos[2], quantum anomalies in molecular systems[3], experimental search for the smallest stable multiply charged anions[4, 5], stability of atoms and molecules in external fields[6, 7], stability of exotic atoms[8], etc.

In general, the energy is non analytical as a function of the Hamiltonian parameters or a bound-state does not exist at the threshold energy (see below). Therefore technical problems appear when standard approximations like perturbation theory, nonlinear variational calculations or Rayleigh-Ritz method are used to study near-threshold properties. Recently, a finite size scaling (FSS) theory for the study of near-threshold properties in quantum few-body problems has been developed (for a review, see Ref. [9]).

FSS methods have been used in many areas of physics. Starting from Fisher FSS theory in statistical mechanics[10], these methods have been widely applied in transfer matrix calculation, Monte Carlo simulations, conformal field theories and polymer physics (for reviews with theoretical background and several applications, see Ref. [11, 12]).

FSS theory is a powerful tool to study critical phenomena of atomic and molecular systems. In this context, "critical" means the point where a bound state is absorbed or degenerates with the continuum. In previous works, *finite size* corresponds to the number of elements of a complete basis set used in a truncated Rayleigh-Ritz expansion of an exact bounded eigenfunction of a given Hamiltonian. This scaling was successfully applied to the calculation of critical parameters and exponents of one-body problems[13–15], two-electron atoms[13, 16], three-electron atoms[17, 18], diatomic molecules[19], three-body Coulomb systems[20], etc.

In this paper, we present a new FSS approach for the calculation of critical parameters and critical exponents of quantum few-body problems. In this case, FSS is done over a spatial variable. The approach does not require basis set expansions as other FSS methods. This point is crucial because the scaling is applicable to other kinds of critical points, like virtual-resonances transitions, where eigenfunctions are not bounded[21].

We will develop the spatial FSS (SFSS) approach for one body three-dimensional central potentials. We consider a one-parameter spherically symmetric potential. In atomic units the Hamiltonian is

$$\mathcal{H}(\lambda;\vec{x}) \;=\; -\frac{1}{2}\nabla^2 \,+\, \lambda\, V(r)\;, \tag{1}$$

where the potential $V(r)$ is assumed negative in some region and $\lim_{r\to\infty} V(r) = 0$, in order to guarantee that Hamiltonian (1) has at least one bound state for large values of λ.

As usual[22], defining $\Psi(\lambda;\vec{x}) = Y_l^m(\theta,\phi)\, u(\lambda;r)/r$, the radial wave function $u(\lambda;r)$ satisfies the reduced Schrödinger equation

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} \,+\, V_{eff}(\lambda;r)\right] u(\lambda;r) \;=\; -E(\lambda)\, u(\lambda;r)\;, \tag{2}$$

where the effective potential includes the centrifugal term

$$V_{eff}(\lambda;r) \;=\; \lambda\, V(r) \,+\, \frac{l(l+1)}{2r^2}\;, \tag{3}$$

$E(\lambda) > 0$ for bound states and $u(\lambda;r)$ obeys the boundary condition $u(\lambda;r=0) = 0$.

We assume that eq. (2) has at least one bound state with energy $E(\lambda)$ that presents a critical point at $\lambda = \lambda_c > 0$. As in previous works we will define critical exponents characterizing the near threshold behavior[9]. In particular, for the energy we define the critical exponent α by the relation

$$E(\lambda) \,\sim\, (\lambda \,-\, \lambda_c)^{\alpha} \quad \text{for } \lambda \to \lambda_c^+\;. \tag{4}$$

The near-threshold properties of other magnitudes, like the size of the system [23] and the particle density [15], are related to the energy, and therefore critical exponents for these quantities are functions of α.

In case of short range potentials ($\lim_{r\to\infty} r^n V(r) < \infty\ \forall n$), some characteristics of the near threshold behavior of the energy are[24]:

- $S-$waves have $\alpha = 2$, $E(\lambda)$ is analytical in $\lambda = \lambda_c$ and $E(\lambda_c) = 0$ is not an eigenvalue of Hamiltonian (1). For $\lambda < \lambda_c$, the bound state turns into a virtual state.

- $\alpha = 1$ for all $l \geq 1$ eigenvalues. $E(\lambda_c)$ is an eigenvalue and $E(\lambda)$ is not analytical at $\lambda = \lambda_c$. A virtual state also exists for $\lambda \to \lambda_c^+$. The bound and the virtual states collide at $\lambda = \lambda_c$ and a resonance pair appears for $\lambda < \lambda_c$.

Long range potentials may have different critical behavior and consequently, different critical exponents. Moreover, a two-parameter Hamiltonian may have a critical exponent α which can be a continuous function of one of the parameters[25].

We will use the fact that the potential tends to zero for $r \to \infty$ to introduce the scaling length R defining a compact support potential $V_R(\lambda; r)$ as

$$V_R(\lambda; r) \ = \ \begin{cases} V_{eff}(\lambda; r) & \text{if } \ r \leq R \\ 0 & \text{if } \ r > R \ . \end{cases} \tag{5}$$

For this potential, the reduced Schrödinger equation for $S-$waves becomes

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} \ + \ V_R(\lambda; r) \right] u_R(\lambda; r) \ = \ -E_R(\lambda) \, u_R(\lambda; r)/, , \tag{6}$$

with the boundary conditions $u_R(\lambda; r = 0) = 0$, and $d \ln(u_R(\lambda; r))/dr$ continuous at $r = R$.

Eq. (6) can be solved, with a arbitrary precision, using the Siegert method[26]. Therefore, Siegert method is a very accurate numerical approach to solve the Schrödinger equation (2). Consequently the scaling ansatz also gives a powerful numerical tool, useful for calculating critical parameters related with bound states, resonances and virtual states[27, 28].

As we pointed out before, $S-$waves of a Hamiltonian with a compact support potential have critical exponent $\alpha = 2$ and the energy is analytical at the critical point. Therefore, near the critical point $\lambda = \lambda_R$ of eq.(6), the asymptotic form of the ground state energy is [24]

$$E_R(\lambda) \ \sim \ a_R \, (\lambda - \lambda_R)^2 \quad \text{for} \ \ \lambda \to \lambda_R^+ \quad ; \quad a_R \neq 0 \quad \forall R < \infty \ . \tag{7}$$

We will assume that the ground state energy of the Hamiltonian in eq.(1) has an asymptotic behavior defined by eq.(4) with critical exponent $\alpha \neq 2$. The main hypothesis of the scaling ansatz, that make the different values of α compatible, is that the coefficient a_R (analytical for finite values of R), has to develop a singularity at the exact critical value λ_c for $R \to \infty$. This singularity is assumed of the form

$$a_R \ \sim \ \frac{a}{(\lambda_c - \lambda_R)^\eta} \quad \text{for} \quad R \to \infty \ , \tag{8}$$

where a is a positive constant. Then, the asymptotic behavior of the energy near λ_R for large values of R is

$$E_R(\lambda) \;\sim\; a\,\frac{(\lambda-\lambda_R)^2}{(\lambda_c-\lambda_R)^\eta}\;. \tag{9}$$

Therefore, we can evaluate the asymptotic expression of the energy $E_R(\lambda)$ in eq. (9) at $\lambda=\lambda_c$, giving

$$E_R(\lambda_c) \;\sim\; a\,(\lambda_c-\lambda_R)^{2-\eta}\;. \tag{10}$$

This relation gives the correction to the finite size critical exponent. The exact critical exponent α for Hamiltonian in eq. (1) is then obtained as

$$\alpha \;=\; 2-\eta\;. \tag{11}$$

In a different context, in statistical mechanics theory of critical phenomena, corrections to classical exponents are calculated using systematic series of mean field approximations [29].

Usually, η, λ_c, λ_R and a in eqs. (10) and (11) are unknown parameters. In order to calculate them, we will study asymptotic expressions of diverse magnitudes for large values of the cutoff radius R.

We assume that the critical parameter for eq. (6) tends to the exact critical parameter of Hamiltonian in eq. (1) for large values of R in the form

$$\lambda_R \;\sim\; \lambda_c-\frac{\delta}{R^\mu} \quad \text{for } \; R\to\infty\;, \tag{12}$$

where δ is a positive constant, and μ is an unknown scaling exponent. Substituting λ_R in eq. (10), the energy at $\lambda=\lambda_c$ satisfies

$$E_R(\lambda_c) \;\sim\; \frac{cons.}{R^{(2-\eta)\mu}} \quad \text{for} \quad R\to\infty\;. \tag{13}$$

Calculating the energy for two different values of R, and taking the logarithm of the quotient we obtain

$$\ln\left(\frac{E_{R_1}(\lambda_c)}{E_{R_2}(\lambda_c)}\right) \;\sim\; (2-\eta)\mu\ln\left(\frac{R_2}{R_1}\right) \quad \text{for} \quad R_1,\,R_2\to\infty\;. \tag{14}$$

In order to obtain a second relation between the exponents η and μ, we use the Hellmann-Feynman theorem and eq. (9), resulting

$$\left\langle \frac{\partial \mathcal{H}_R}{\partial \lambda} \right\rangle = \frac{\partial E_R(\lambda)}{\partial \lambda} \sim 2a \frac{(\lambda - \lambda_R)}{(\lambda_c - \lambda_R)^\eta} . \tag{15}$$

Analogously as we did with the energy, we calculate this quantity for two different values of R, and we take the logarithm of the quotient to obtain

$$\ln \left(\frac{\frac{\partial}{\partial \lambda} E_{R_1}(\lambda)}{\frac{\partial}{\partial \lambda} E_{R_2}(\lambda)} \right) \Bigg|_{\lambda=\lambda_c} \sim (1-\eta)\mu \ln \left(\frac{R_2}{R_1} \right) \quad \text{for} \quad R_1,\ R_2 \to \infty . \tag{16}$$

Now, we can eliminate the exponent μ defining a function $\Gamma(R_1, R_2; \lambda)$ as

$$\Gamma(R_1, R_2; \lambda) = \ln \left(\frac{E_{R_1}(\lambda)\ (\frac{\partial}{\partial \lambda} E_{R_2}(\lambda))^2}{E_{R_2}(\lambda)\ (\frac{\partial}{\partial \lambda} E_{R_1}(\lambda))^2} \right) \Big/ \ln \left(\frac{E_{R_1}(\lambda)\ \frac{\partial}{\partial \lambda} E_{R_2}(\lambda)}{E_{R_2}(\lambda)\ \frac{\partial}{\partial \lambda} E_{R_1}(\lambda)} \right) . \tag{17}$$

In particular, for $\lambda = \lambda_c$ and $R_1,\ R_2 \to \infty$, we have

$$\Gamma(R_1, R_2; \lambda_c) = \eta , \tag{18}$$

independent of the values of R_1 and R_2.

Now, if we plot $\Gamma(R_i, R'_i; \lambda)$ vs. λ, for $i = 1, \cdots, N$, where $\{R_i, R'_i\}$ is an arbitrary set of pairs of (large) values of R, eq. (18) shows that all these curves will intersect at the same point $\lambda = \lambda_c$. The value of the function Γ, at this point, is the critical exponent η. Actually, this result is asymptotic and we will have a set of values $\{\lambda_c^{(i)}, \eta^{(i)}\}_{i=1,N}$. Final estimations of (λ_c, η) have to be obtained performing an extrapolation of the data for $1/R \to 0$.

Usually, the FSS parameter is a discrete variable, like the width of a finite lattice, or the number of functions in a basis-set expansion, etc. In these cases, the most accurate results are obtained looking for intersections of curves with minimum difference between the FSS parameters [9, 11]. In our case the parameter R is a real variable. Therefore, the minimum difference between parameters is given by the limit $R_2 \to R_1$. This limit introduces derivatives of the functions $E_R(\lambda)$ and $\partial E_R(\lambda)/\partial \lambda$ with respect to R. In practice, the derivatives have to be calculated numerically. For this reason, it is convenient to use a finite difference $R_2 - R_1$, fixed by numerical stability studies.

As a test, we apply SFSS to a Hamiltonian with support compact potential and non zero value of the angular momentum l. In this case, the exact critical exponent is $\alpha = 1$[24]. An asymptotic analysis can be done analytically, and the exact scaling exponents are $\eta = 1$ and $\mu = 3$.

The Siegert method[26] assumes that the potential vanishes outside a sphere of radius R and gives the exact solution of eq. (6). A Siegert state is a solution of the Schrödinger eq. (6), defined for $0 \leq r \leq R$ with the boundary conditions $u_R(\lambda; r = 0) = 0$ and $u_R(\lambda; r = R) = -k u'_R(\lambda; r = R)$, where $k = +(-)\sqrt{2E}$ for bound (virtual) states.

In particular, we study the usual spherical square well of width $r_0 = 1$ and depth equal to λ. We apply the Siegert method to states of angular momentum $l = 1$. The exact value of the critical point for the lowest energy $l = 1$ state is $\lambda_c = \pi^2/2 \simeq 4.9348022$.

The usual technique is to perform a numerical integration of eq. (6) using boundary conditions at $r = 0$ and looking for the eigenvalue $E_R(\lambda)$ by a shooting method applied iteratively until the boundary condition at $r = R$ is satisfied. In our example, the transcendental equation for the energy is known for all values of R and neither numerical integration, nor extrapolation are needed.

In figure 1, we show $\Gamma(R, R+1; \lambda)$ against λ for $R = 10, 20, \cdots, 100$ for the lowest energy $l = 1$ bound state. As the asymptotic result in eq. (18) predicts, the curves intersect at (approximately) the same point. Numerical values for the critical parameters as a function of R were obtained from the relation

$$\Gamma(R-1, R; \lambda_c^{(R)}) \;=\; \Gamma(R, R+1; \lambda_c^{(R)}) \;=\; \eta^{(R)} \,. \tag{19}$$

In figure 2, the critical point $\lambda_c^{(R)}$ for finite values of R is plotted against $1/R$. Virtual state solutions of eq.(18) exist for $R \geq 12$. The insert magnifies the region where both, bound state (solid curve) and virtual state (dashed curve), solutions exist.

Finally, $\eta^{(R)}$ against $1/R$ is shown in figure 3. Note the maximum at $R \simeq 25$. This behavior is related to the large coefficient in the correction to the dominant asymptotic term. As usual in FSS[9, 11], the convergence process is faster for the critical parameter calculation, than for the critical exponent calculation.

In summary, we have developed a SFSS approach to study the critical behavior of bound and virtual states of the radial Schrödinger equation. The scaling is done introducing a cutoff radius in the potential. This cutoff radius changes the critical exponent of the energy, but, for large values of the cutoff radius, the asymptotic behavior of FSS functions is dominated by the exact critical exponent. The method gives accurate values for critical parameters and critical exponents.

The SFFS ansatz is not based on variational principles and does not use basis set expansions. Therefore, it might be a powerful tool to study bound-virtual-resonances transitions and other analytical properties of the complex energy plane. Work is in progress in this direction.

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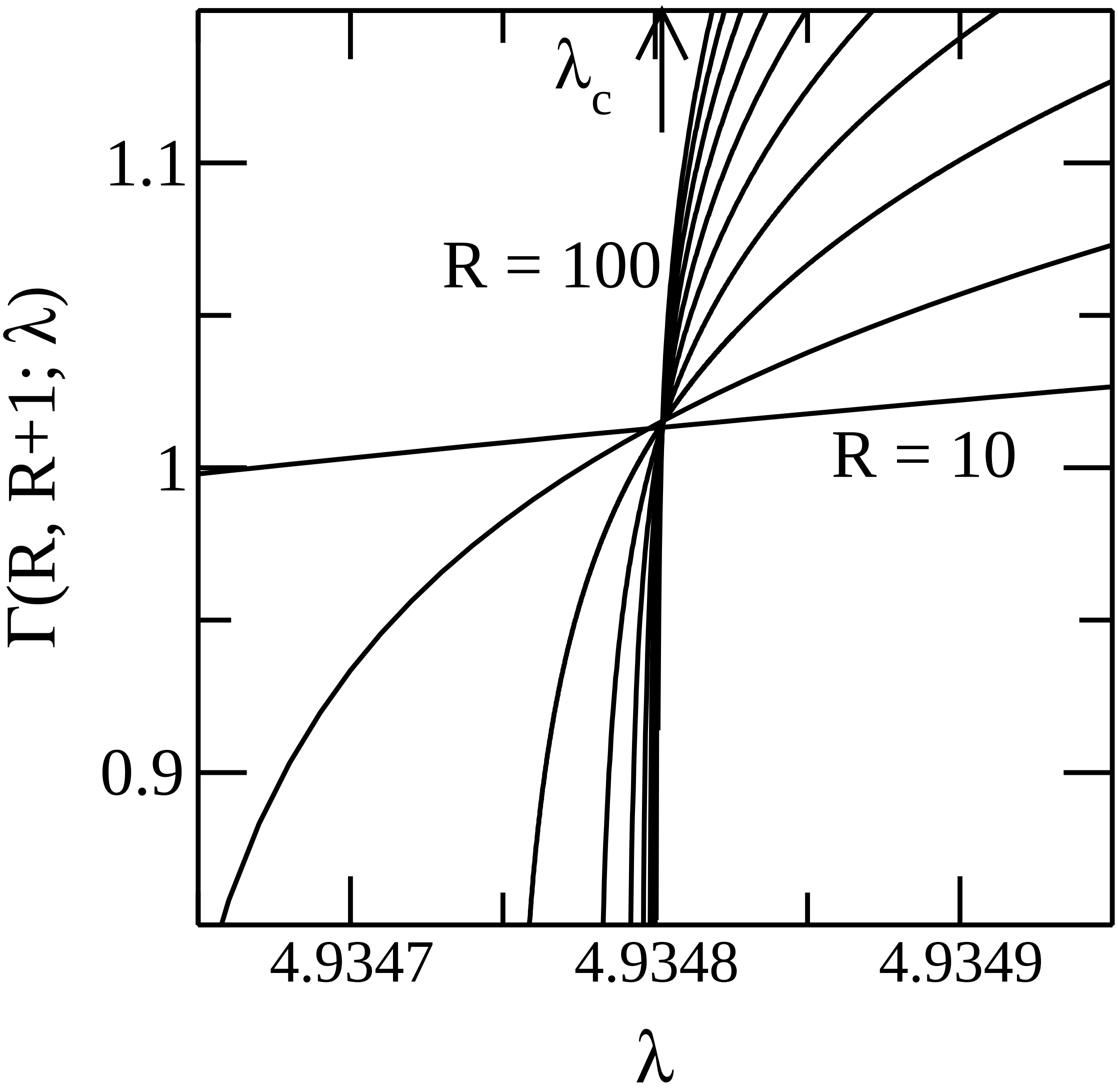

FIG. 1: $\Gamma(R, R+1; \lambda)$ as a function of λ for the lowest energy $l = 1$ bound state of the spherical square well potential for values of $R = 10, 20, \cdots 100$. The arrow indicates the exact value of $\lambda_c = \pi^2/2$.

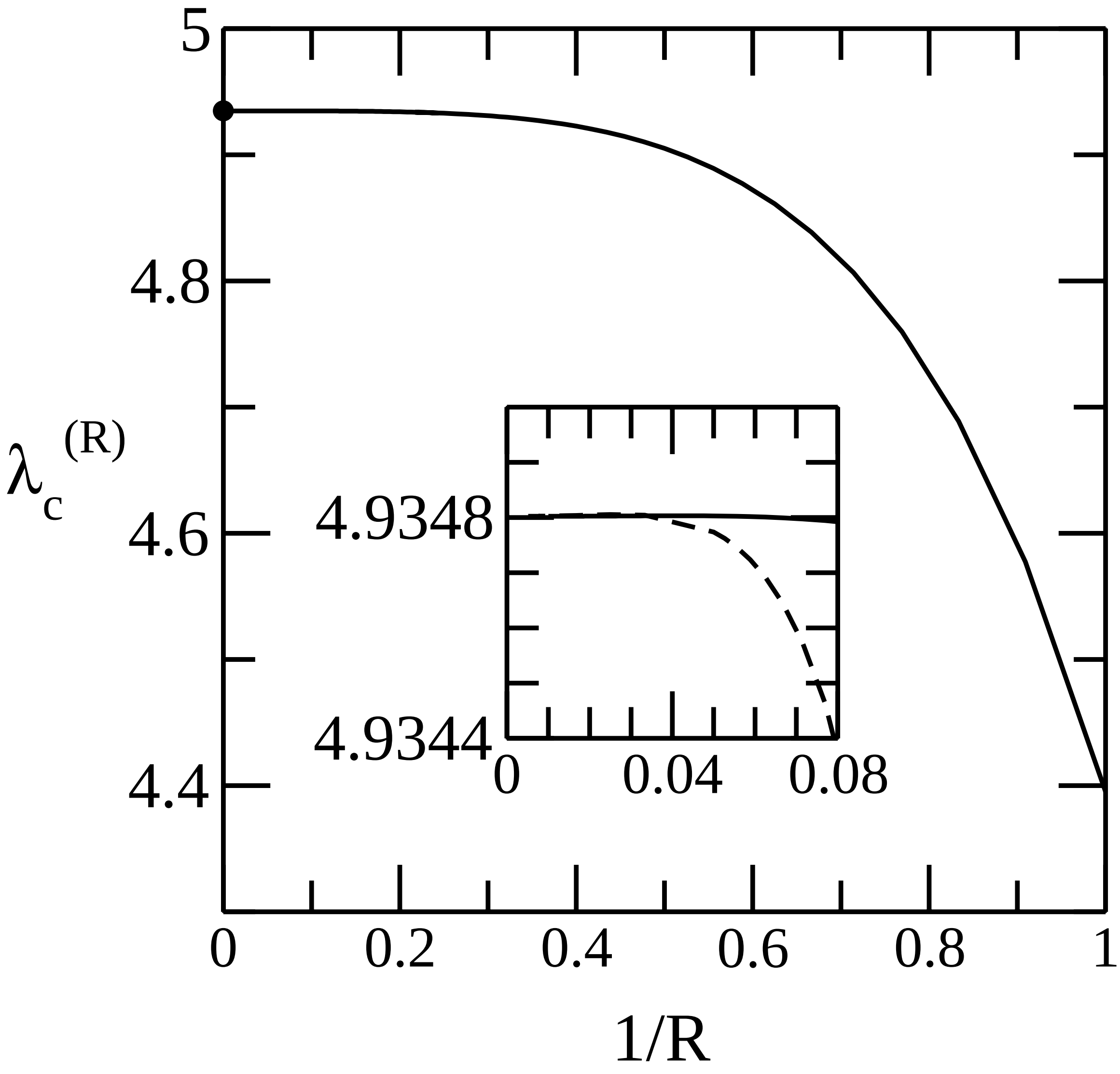

FIG. 2: $\lambda_c^{(R)}$ vs. $1/R$ for the lowest energy $l = 1$ bound state of the spherical square well potential. The dot indicates the exact value of $\lambda_c = \pi^2/2$. The insert shows bound-state (solid line) and virtual-state (dashed line) values of $\lambda_c^{(R)}$.

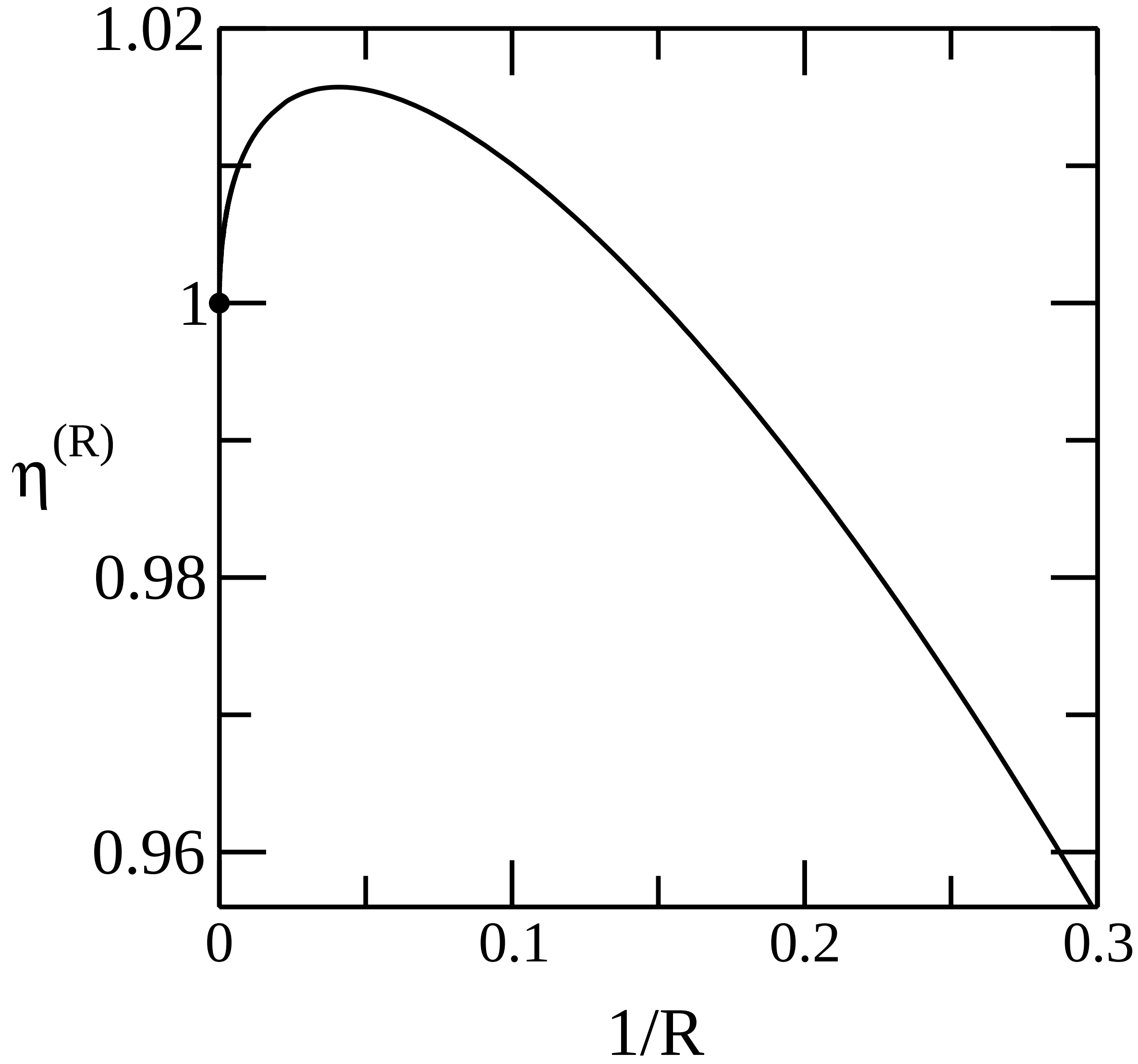

FIG. 3: $\eta^{(R)}$ vs. $1/R$ for the lowest energy $l = 1$ bound state of the spherical square well potential. The exact value of $\eta = 1$ is also shown by a dot.