Generalisation of the envelope theory for systems with different particles

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The envelope theory is a method to easily obtain approximate, but reliable, solutions for some quantum many-body problems. Quite general Hamiltonians can be considered for systems in D dimensions, and the scope of the method can span many fields of Physics. Recently, the method has been extended to treat systems with different particles, with good results for power-law potentials and relativistic kinematics.

Introduction

The Schrödinger equation $(-\frac{1}{2m}\nabla^2 + V)\psi = E\psi$, with $\hbar = 1$, is the equation of motion for quantum systems for one particle or for a relative motion. When solved, it gives access to the eigenvalues E and eigenfunctions ψ of the system. Only some Hamiltonians H like the harmonic oscillator or the hydrogen atom can be solved analytically. Some techniques like supersymmetric quantum mechanics [1] can be used to determine if this is the case. Otherwise, the equation can be numerically solved with many methods.

The Schrödinger equation can also be written for systems with many particles. We will consider the following N-body Hamiltonian

$$H = \sum_{i=1}^{N} T_i(p_i) + \sum_{i<j=2}^{N} V_{ij}(r_{ij}), \qquad (1)$$

where T_i is an arbitrary kinetic energy, with some constraints [2], depending on $p_i = |\boldsymbol{p}_i|$, and V_{ij} is a two-body potential depending on $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$. In the following, all computations will be performed in the centre of mass frame. Only a handful of many-body systems can be solved analytically such as the harmonic oscillator [3] or the Calogero model at $D = 1$ dimension [4]. Otherwise, numerical methods need to be used. We can cite e.g. the oscillator basis expansion [5], the gaussian basis expansion [6], the hyperspherical harmonic expansion [7] or the Lagrange-mesh method [8]. These methods can be very accurate, but they are generally very heavy to implement and need long computation times. In this article, we would like to present the method of the envelope theory (ET).

The key element of the ET is the fact that the complete solution of an N-body harmonic oscillator Hamiltonian, says H_{ho}, exists as stated above. Then, the idea is to build an auxiliary Hamiltonian, $\tilde{H} = H_{\text{ho}} + B$, where B is a function unequivocally determined from the structure of H. By using an extremisation procedure, eigenvalues of $\tilde{H}$ can be rendered very close to those of H. The procedure to build $\tilde{H}$ and compute the approximate solutions of H is described in the following sections. The big advantage of the method is that its computational cost is independent of the number of particles N, which is especially useful when the number of particles can be arbitrary large as for baryons in the large-N formulation of QCD [9–12]. The ET has

been first developed to treat systems with identical particles (bosons or fermions) [13, 14]. In some favourable situations, analytical upper or lower bounds can be computed. Recently, the method has been extended to treat systems with different particles [15, 16]. This generalisation opens new domains of applicability of the method such as in hadronic physics with the study of hybrid baryons, which are exotic states composed of 3 quarks (or N_c quarks with the gauge group $SU(N_c)$) and a constituent gluon.

Previous results for identical particles

We would like first to present some previous results computed with the ET to show the interest of the method. We will explain the construction of the method itself in the next sections.

At first, let us consider a non-relativistic kinematic energy $T(p) = p^2/2m$ with a Coulomb potential $V(r) = -g/r$ at $D = 3$. The ET gives the following analytical result for the bosonic ground state (BSG) [17]:

$$E_{\text{ET}} = -\frac{N^2(N-1)}{4}\frac{mg^2}{(\phi+1)^2}.$$

As we can see, the number of particles N appears as a simple parameter. We will discuss later the meaning of the parameter ϕ. When $\phi = 2$, we can show that the ET gives an upper bound as we can see in Fig. 1. Our approximate solution also matches the general behaviour of the exact solution. The ET can also be used to compute eigenfunctions and so observables, as shown in Fig. 1 for the mean relative distance $\langle r \rangle$.

Secondly, we consider the same non-relativistic kinematics but with a central Gaussian potential $V(r) = -V_g e^{-x^2/a^2}$ at $D = 1$. The approximate eigenvalue for the BGS is given by [14]:

$$E_{\text{ET}} = -\frac{N(N-1)}{2} V_g Y^2 \frac{1+2W_0(Y)}{W_0(Y)^2},$$
$$\text{with } Y = -\frac{1}{2a\sqrt{2mV_gN}},$$

where the Lambert function $W_0(z)$ is the inverse of ze^z. This approximation as been compared to very accurate results up to 100 bosons as we can see in Fig. 2. Computing the energy for such a large number of particles is not a problem for the ET. The accuracy is also very good with a relative error around 0.05% for $N = 100$. Similar results have been found for the same system at $D = 3$ up to $N = 20$ [17].

Harmonic oscillator

As mentioned in the Introduction, the only many-body system that can be solved analytically at D dimensions is the harmonic oscillator

$$H_{\text{ho}} = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i<j=2}^{N} k_{ij} r_{ij}^2. \tag{2}$$

The eigenvalues can be obtained by the diagonalisation of a matrix of order $(N-1)$ [3, 20–22].

It is useful to define the following global quantum number for a set of M identical particles

$$Q(M) = \sum_{k=1}^{M-1} (2n_k + l_k + D/2), \tag{3}$$

where $\{n_k, l_k\}$ are the quantum numbers associated with the internal Jacobi variables. This global quantum number allows us to specify if we have a system of bosons or fermions, or if we want the ground state or excited states. Its computation is not easy but some values are given in [14, 15]. For instance, for the BGS we have a simple value $Q_{\text{BGS}} = (M-1)\frac{D}{2}$.

If we specify (2) for a system composed of N identical particles, the diagonalisation procedure gives the following eigenvalue

$$E_{\text{ho}} = Q(N)\sqrt{\frac{2Nk}{m}}. \tag{4}$$

On the other hand, if we specify (2) for a system composed of N_a identical particles of type a plus a different one of type b, we obtain the more complex solution

$$E_{\text{ho}} = Q(N_a)\sqrt{\frac{2}{m_a}(N_a k_{aa} + k_{ab})} + Q(2)\sqrt{\frac{2(N_a m_a + m_b)}{m_a m_b} k_{ab}}. \tag{5}$$

A generalisation of this formula has also been determined for a system of $N_a + N_b$ particles [15]. These exact solutions will be the starting point of the ET.

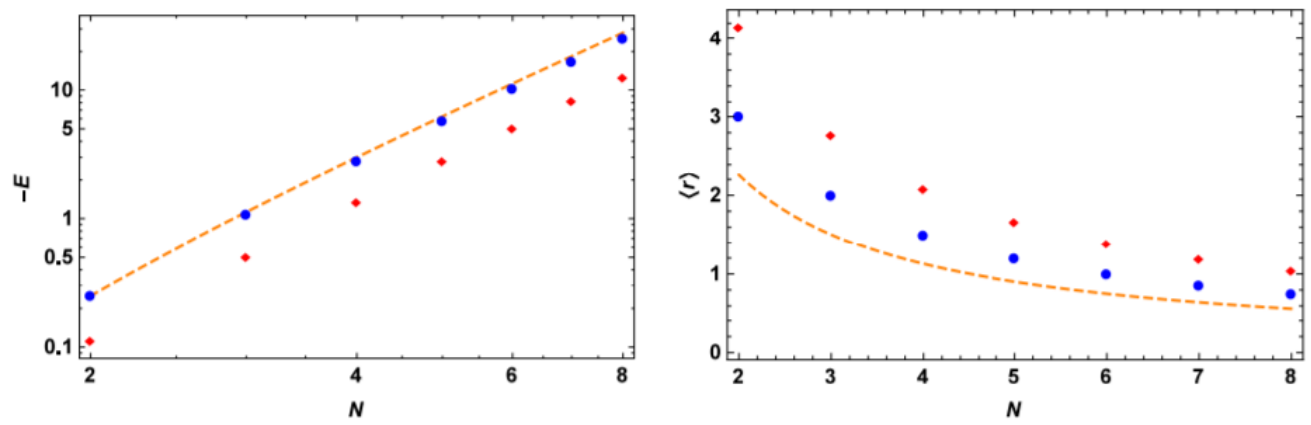

Figure 1: *Binding energies $-E$ (left) and mean relative distances $\langle r \rangle$ (right) of self-gravitating bosons for $m = g = 1$: exact results (circle) [18], ET results for $\phi = 2$ (diamond) and improved ET results for $\phi = 1$ (dashed line for visibility).*

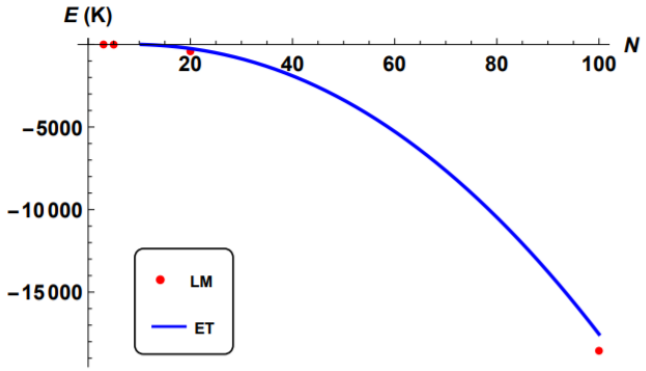

Figure 2: *Energies in K for the Gaussian potential for $1/m = 43.3\ (a.u.)^2$, $a = 1$ a.u. and $V_g = 5.6$ K: accurate results (dot) from Lagrange-mesh (LM) method [19] and upper bounds computed with the ET (solid line for visibility).*

Construction of the envelope theory

The idea of the ET is to replace the original Hamiltonian H with the following auxiliary Hamiltonian [23–26], where $\{\alpha\} = \{\{\mu_i\}, \{\rho_{ij}\}\}$,

$$\tilde{H}(\{\alpha\}) = \sum_{i=1}^{N} \left[\frac{p_i^2}{2\mu_i} + T_i(G_i(\mu_i)) - \frac{G_i^2(\mu_i)}{2\mu_i} \right] + \sum_{i<j=2}^{N} \left[\rho_{ij} r_{ij}^2 + V_{ij}(J_{ij}(\rho_{ij})) - \rho_{ij} J_{ij}^2(\rho_{ij}) \right], \tag{6}$$

where G and F are functions entirely determined by the original Hamiltonian [15], and $\{\alpha\}$ are auxiliary parameters to determine later. The number of parameters can be reduced thanks to the symmetries of the system. Indeed, we can show that for a set of identical particles there is only one parameter μ and one parameter ρ. For $N_a + 1$ particles, we have thus four parameters μ_a, μ_b, ρ_{aa} and ρ_{ab}.

Another form of (6) is

$$\tilde{H}(\{\alpha\}) = H_{\text{ho}}(\{\alpha\}) + B(\{\alpha\}), \tag{7}$$

where B is a function obtained by subtracting the harmonic oscillator contributions from (6). An eigenvalue of (6) is thus

$$\tilde{E}(\{\alpha\}) = E_{\text{ho}}(\{\alpha\}) + B(\{\alpha\}), \tag{8}$$

where E_{ho} is the eigenvalue of the harmonic oscillator (either (4) or (5) for the two particular systems presented above). The principle of the method is to search for the set of parameters $\{\alpha_0\} = \{\{\mu_{i0}\}, \{\rho_{ij0}\}\}$ such that

$$\left.\frac{\partial \tilde{E}}{\partial \mu_i}\right|_{\{\alpha_0\}} = \left.\frac{\partial \tilde{E}}{\partial \rho_{ij}}\right|_{\{\alpha_0\}} = 0 \qquad \forall\ i, j. \tag{9}$$

After solving (9), we obtain the desired approximate energy E_{ET} by substituting the set $\{\alpha_0\}$ back to (8), $\tilde{E}(\{\alpha_0\}) = \tilde{E}_0$. When (8) can be written analytically, equations (9) correspond to a simple optimisation problem which can be done analytically or numerically.

An interesting property of the method is that, when optimisation equations (9) are fulfilled, each respective parts of Hamiltonians H and $\tilde{H}(\{\alpha_0\})$ will be tangent at least at one point [15, 24], thus forming an envelope and giving the name to the method. When some conditions are fulfilled, lower or upper bounds are possible, which was the case for the examples given above.

Compact equations

It has been shown that solving (9) for a system of $N_a + 1$ particles is equivalent to solve the following set of five compact equations [27]

$$\tilde{E}_0 = N_a T_a\left(p'_a\right) + T_b\left(P_0\right) + C^2_{N_a} V_{aa}\left(r_{aa}\right) + N_a V_{ab}\left(r'_0\right), \tag{10a}$$

$$N_a T'_a(p'_a)\frac{p_a^2}{p'_a} = C^2_{N_a} V'_{aa}(r_{aa}) r_{aa} + \frac{N_a - 1}{2} V'_{ab}(r'_0)\frac{r_{aa}^2}{r'_0}, \tag{10b}$$

$$\frac{1}{N_a} T'_a(p'_a)\frac{P_0^2}{p'_a} + T'_b(P_0)P_0 = N_a V'_{ab}(r'_0)\frac{R_0^2}{r'_0}, \tag{10c}$$

$$Q(N_a) = \sqrt{C^2_{N_a}}\, p_a r_{aa}, \tag{10d}$$

$$Q(2) = P_0 R_0, \tag{10e}$$

with ${p'_a}^2 = p_a^2 + \frac{P_0^2}{N_a^2}$ and ${r'_0}^2 = \frac{N_a - 1}{2N_a} r_{aa}^2 + R_0^2$.
These equations are called compact because all the relevant variables appear in five equations giving the definition of the energy (10a), the equations of motion (10b,10c) and the rules for the quantisation (10d,10e). Moreover, the uninteresting auxiliary parameters and functions are not present. Equations (10) can also be easily implemented and solved as follow: first we compute the variables p_a, P_0, r_{aa} and R_0 by solving (10b-10e). Then we substitute their values in (10a) to compute the energy $\tilde{E}_0$.
There are good reasons to prefer the compact equations (10) over the optimisation equations (9). First, the quantities p_a, P_0, r_{aa} and R_0 give direct access to more interesting expectation values than $\{\alpha_0\}$. Secondly, these equations have a nice semiclassical interpretation [13]. Thirdly, it is possible to improve the ET starting from these equations [28], which is the main motivation to write these equations.
The compact equations for a system of $N_a + N_b$ particles have also been determined in [27].

Improvement of the method

One reason for inaccuracies in the ET is the strong degeneracy of the harmonic oscillator eigenvalue. For systems with all identical particles, it has been shown [17] that the modification of $Q(M)$ in the following way

$$Q_\phi(M) = \sum_{k=1}^{M-1}\left(\phi n_k + l_k + \frac{D + \phi - 2}{2}\right) \tag{11}$$

can allow a noticeable improvement of the ET results when $D \geq 2$ (this is why the parameter ϕ is not introduced in the previous example at $D = 1$). The parameter ϕ takes its origin from [29] where an effective quantum number for centrally symmetric 2-body systems has been introduced. The modified quantum number (11) is a generalisation to N-body systems. We retrieve the original ET when $\phi = 2$.
The value of ϕ can be determined either by fitting some exact solutions, or by using the ET in combination with a generalisation of another method, the dominantly orbital state method (DOSM) [28]. The DOSM has been initially developed for 2-body systems but, thanks to the compact equations of the ET, it can be generalised to N-body systems. For instance, for the first example given in the second section, computations give the simple value $\phi = 1$. Fig. 1 clearly shows an improvement of the accuracy for the energy.
This improvement procedure has been recently generalised for systems with $N_a + 1$ particles [16] where we need to introduce two parameters ϕ_a and ϕ_b since we have two global quantum numbers in (5).

Results

Now that the method and the equations have been established, we will check the accuracy by computing the BGS for a variety of different Hamiltonians. ET results are given in [15] and improved results (IET) in [16]:

1. $D = 3$ Hamiltonian for a three-body system of ultra-relativistic harmonic oscillators (arbitrary units)

$$H = \sum_{i=1}^{3} |p_i| + r_{12}^2 + \lambda \sum_{i=1}^{2} r_{i3}^2. \tag{12}$$

The ET ($\phi = 2$) predicts an upper bound as we can see in the table below.

	Exact [30]	ET	IET
$\lambda = 0.1$	5.288	5.597 (5.8)	5.307 (0.4)
$\lambda = 10$	14.506	15.353 (5.8)	14.699 (1.3)

The relative errors in % are indicated between parentheses. With the original ET, the accuracy is around 6% which is great for such a simple method as the ET. When the improvement is considered, the relative errors drop to 1% or less.

2. $D = 3$ Hamiltonian for a three-body system with power-law potential (arbitrary units)

$$H = \sum_{i=1}^{2} \frac{p_i^2}{2} + \frac{p_3^2}{2m} + \frac{1}{2}\mathrm{sgn}(\beta) \sum_{i<j=2}^{3} r_{ij}^{\beta}. \quad (13)$$

The ET ($\phi = 2$) predicts an upper bound for $\beta < 2$ and a lower bound when $\beta > 2$. When $\beta = 2$, we retrieve the harmonic oscillator and so the ET gives the exact result. In the results below we took $m = 0.2$.

β	Exact [31]	ET	IET
-1	-0.1398	-0.0645 (54)	-0.1316 (5.9)
0.1	1.9452	1.9804 (1.8)	1.9489 (0.2)
1	4.9392	5.2278 (5.8)	4.9687 (0.6)
3	9.7389	8.9925 (7.7)	9.6703 (0.7)

The relative accuracy obtained by the ET is better than 8%, except for the Coulomb case. The improvement is again quite large with the IET, even if its magnitude seems quite unpredictable. Similar results have been found for $m = 5$ [16].

3. Hamiltonian of atoms (a.u.)

$$H = \frac{1}{2}\sum_{i=1}^{N_e} p_i^2 + \frac{1}{2m}p_N^2 - Z\sum_{i=1}^{N_e}\frac{1}{r_{iN}} + \sum_{i<j=2}^{N_e}\frac{1}{r_{ij}}. \quad (14)$$

Due to the mixing of attractive and repulsive potentials, the ET has no variational character. Binding energies below are given in eV.

	ET	IET	Exp.
^{4}He	33	47	79
^{6}Li	66	95	203
^{6}Li$^+$	85	123	198

Unlike the previous examples, the accuracy of the ET is quite bad, even with the improvement procedure. We have here an example of the limitation of the method. It is not clear why for such systems the accuracy of the ET is not good, but the singularity of the Coulomb potential is a possible explanation. More research have to be conducted to predict the accuracy of the ET.

Conclusion

In this article, we have explained the main properties of the envelope theory, with a focus for systems with identical particles plus a different one. The approximate energies can be computed with either optimisation equations, or with a set of five compact equations. The accuracy is tested with three different systems: relativistic oscillators, power-law potential and atoms. As in the case of identical particles, fairly good results can be obtained with the original envelope theory for some kinds of potentials, and an improvement of the accuracy can always be obtained thanks to the IET. We have also seen some limitations of the method. Even if the envelope theory method can lack accuracy in certain cases, it is remarkably easy to implement. The low computational cost of this method and the fact that the computational cost is independent of the number of particles make it worthwhile. With the generalisation presented above, new domains of applicability are open, especially in hadronic physics where the method is proven to be useful as mentioned in the Introduction [9–12, 32]. Other applications of the method could be found in the estimation of the binding energies of systems such as nuclei or clusters of cold atoms for which ab-initio calculations are already available, as for instance in [33,34], or for more particular quantum problems [35]. The method can also be simply used to check other, more accurate, methods.

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