Envelope theory for systems with different particles

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Abstract

The eigensolutions of many-body quantum systems are always difficult to compute. The envelope theory (ET) is a method to easily obtain approximate, but reliable, solutions in the case of identical particles. The big advantage of the method is that its computational cost is independent of the number of particles N. It is extended here to treat systems with different particles (bosons or fermions). The accuracy is tested for several systems composed of identical particles plus a different one.
With the ET, it is possible to treat the following Hamiltonians

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

with $p_i = |\boldsymbol{p}_i|$ and $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$. All computations are performed in the centre of mass frame $\boldsymbol{P} = \sum_{i=1}^{N} \boldsymbol{p}_i = \boldsymbol{0}$. One-body potentials can also be considered.

Previous results for identical particles

Coulomb potential $V(r) = -g/r$ with a non-relativistic kinematics $T(p) = p^2/2m$ for $D = 3$ for the bosonic ground state (BSG).

$\Rightarrow$ approximate result [1]: $E_{\text{ET}} = -\frac{N^2(N-1)}{4}\frac{mg^2}{(\phi+1)^2}$ with $\phi = \begin{cases} 2 \text{ for an upper bound} \\ 1 \text{ for improved ET} \end{cases}$

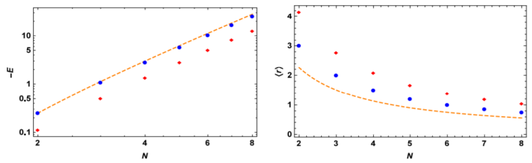

Fig. 1: ET results for $\phi = 2$ (diamond), improved ET results for $\phi = 1$ (line) and exact results (dot) for the energy (left) and mean relative distance (right).

Harmonic oscillator

The key element of the ET is the fact that the complete solution of an N-body harmonic oscillator Hamiltonian

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

can be obtained by the diagonalization of a matrix of order $(N-1)$ [2]. It is useful to define

$$Q(N) = \sum_{i=1}^{N} (2n_i + l_i + D/2)\,. \tag{3}$$

For a system composed of N_a identical particles a plus a different one b, we obtain

$$E_{\text{ho}} = Q(N_a)\sqrt{\frac{2}{m_a}(N_a k_{aa} + k_{ab})} + Q(2)\sqrt{\frac{2(N_a m_a + m_b)}{m_a m_b}k_{ab}}. \tag{4}$$

The same solution can be found with a clever decomposition of H_{ho} yielding solution for a system with $N_a + N_b$ particles [3]

General properties of the method

Let's build the auxiliary Hamiltonian, with $\{\alpha\} = \{\{\mu_i\}, \{\rho_{ij}\}\}$,

$$\begin{aligned}\tilde{H}(\{\alpha\}) = &\sum_{i=1}^{N}\left[\frac{p_i^2}{2\mu_i} + T_i(G_i(\mu_i)) - \frac{G_i^2(\mu_i)}{2\mu_i}\right] \\ &+ \sum_{i<j=2}^{N}\left[\rho_{ij} r_{ij}^2 + V_{ij}(J_{ij}(\rho_{ij})) - \rho_{ij} J_{ij}^2(\rho_{ij})\right],\end{aligned} \tag{5}$$

Another form is $\tilde{H}(\{\alpha\}) = H_{\text{ho}}(\{\alpha\}) + B(\{\alpha\})$. An eigenvalue of (5) is thus

$$\tilde{E} = E_{\text{ho}}(\{\alpha\}) + B(\{\alpha\}). \tag{6}$$

The principle of the method is to search for the set of parameters $\{\alpha_0\} = \{\{\mu_{i0}\}, \{\rho_{ij0}\}\}$ such that

$$\left.\frac{\partial \tilde{E}}{\partial \mu_i}\right|_{\{\alpha_0\}} = \left.\frac{\partial \tilde{E}}{\partial \rho_{ij}}\right|_{\{\alpha_0\}} = 0 \quad \forall\, i, j. \tag{7}$$

Let's define $\tilde{H}_0 = \tilde{H}(\{\alpha_0\})$ with an eigenstate $|\alpha_0\rangle$ and the eigenvalue $\tilde{E}_0 = \langle\alpha_0|\tilde{H}_0|\alpha_0\rangle$. The latter is an approximate eigenvalue E_{ET} of H.
We can show that, when minimisation equations (7) are fulfilled, each respective parts of Hamiltonians H and $\tilde{H}_0$ will be tangent at least at one point, thus forming an envelope. When some conditions are fulfilled, lower or upper bounds are possible.

Compact equations

It has been shown [4] that solving (7) is equivalent to solve the following set of 5 equations

$$\tilde{E}_0 = N_a T_a(p'_a) + T_b(P_0) + C_{N_a}^2 V_{aa}(r_{aa}) + N_a V_{ab}(r'_0)\,, \tag{8a}$$

$$N_a T'_a(p'_a)\frac{p_a^2}{p'_a} = C_{N_a}^2 V'_{aa}(r_{aa}) r_{aa} + \frac{N_a - 1}{2} V'_{ab}(r'_0)\frac{r_{aa}^2}{r'_0}, \tag{8b}$$

$$\frac{1}{N_a} T'_a(p'_a)\frac{P_0^2}{p'_a} + T'_b(P_0) P_0 = N_a V'_{ab}(r'_0)\frac{R_0^2}{r'_0}, \tag{8c}$$

$$Q(N_a) = \sqrt{C_{N_a}^2}\, p_a r_{aa}, \tag{8d}$$

$$Q(2) = P_0 R_0, \tag{8e}$$

with $p'^2_a = p_a^2 + \frac{P_0^2}{N_a^2}$ and $r'^2_0 = \frac{N_a - 1}{2N_a} r_{aa}^2 + R_0^2$. The resolution of (8) is as follow: first we compute the variables p_a, P_0, r_{aa} and R_0 by solving (8b)-(8e). Then we substitute their values in (8a) to compute the energy $\tilde{E}_0$.
Equations (8) are more interesting than (7) because the variables give direct access to more interesting expectation values than $\{\alpha_0\}$. They have a nice semiclassical interpretation and it is possible to improve the ET starting from these equations.

Improved envelope theory (IET)

For systems with all identical particles, it has been shown that the modification of $Q(N)$ in the following way

$$Q_\phi(N) = \sum_{i=1}^{N}\left(\phi n_i + l_i + \frac{D + \phi - 2}{2}\right) \tag{11}$$

can allow a noticeable improvement of the ET results. The value of ϕ can be determined by using the ET in combination with a generalisation of the Dominantly Orbital State (DOS) method. We retrieve the original ET when $\phi = 2$. This improvement procedure has been recently generalised for systems with $N_a + 1$ particles [5] where we need to introduce two parameters ϕ_a and ϕ_b.

Conclusion

In this work, it is shown that the envelope theory can be extended to treat systems with different particles. The approximate energies can be computed with a set 5 equations. The accuracy is tested with two different systems: relativistic oscillators 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.

Results for different particles

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

$$H = \sum_{i=1}^{3} |p_i| + r_{12}^2 + \lambda \sum_{i=1}^{2} r_{i3}^2. \tag{9}$$

2. Hamiltonian of atoms (a.u.)

$$H = \frac{1}{2}\sum_{i=1}^{N_e} p_i^2 + \frac{1}{2m} p_N^2 - Z\sum_{i=1}^{N_e}\frac{1}{r_{iN}} + \sum_{i<j=2}^{N_e}\frac{1}{r_{ij}}. \tag{10}$$

ET [3] and IET [5] results for the two Hamiltonians (9) and (10):

1. The ET ($\phi = 2$) predicts an upper bound.

	Exact	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]

Tab. 1: BGS eigenvalues of Hamiltonian (9) for two values of λ. The relative errors in % are indicated between square brackets.

2. Due to the mixing of attractive and repulsive potentials, the ET has no variational character.

	ET	IET	Exp.		ET	IET	Exp.
^{4}He	33	47	79				
^{6}Li	66	95	203	^{6}Li$^+$	85	123	198
^{12}C	321	496	1030	^{12}C^{4+}	386	568	882
^{16}O	672	1062	2044	^{16}O^{6+}	707	1047	1611

Tab. 2: Ground state binding energies (in eV) of Hamiltonian (10) for some atoms with two or more electrons.

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