Compact equations for the envelope theory

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(Dated: August 13, 2021)

Abstract 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 composed of an arbitrary number of different particles in D dimensions. In the case of identical particles, a compact set of 3 equations can be written to find the eigensolutions. This set provides also a nice interpretation and a starting point to improve the method. It is shown here that a similar set of 7 equations can be determined for a system containing an arbitrary number of two different particles.

I. INTRODUCTION

The envelope theory (ET) [1–3], also known as the the auxiliary field method, is a technique to compute approximate eigenvalues and eigenvectors of N-body systems in D dimensions. The method, first developed for systems with identical particles [4, 5], has been recently generalized for systems with different particles [6]. The big advantage of this method is that the computation cost is independent from the number of particles. Quite general Hamiltonians can be considered, and the approximate eigenvalues are lower or upper bounds in favorable cases. The method relies on the existence of an exact solution for the N-body harmonic oscillator Hamiltonian [7, 8]. The accuracy of the method has been checked for various three-dimensional systems [9] and one-dimensional systems containing up to 100 bosons [5].

Let us consider the N-body Hamiltonian

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

where T_i is an arbitrary kinetic energy with some constraints [10] and V_{ij} is a two-body potential. We also define $p_i = |\boldsymbol{p}_i|$ and $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$, where $\boldsymbol{r}_i$ and $\boldsymbol{p}_i$ are respectively the position and the momentum of the ith particle. It is assumed in the following that we are always working in the centre of mass (CM) frame, $\boldsymbol{P} = \sum_{i=1}^{N} \boldsymbol{p}_i = \boldsymbol{0}$, and with natural units ($\hbar = c = 1$).

As explained in [6, 11], in the framework of the ET method, Hamiltonian (1) is replaced with an auxiliary Hamiltonian

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

where $\{\alpha\} = \{\{\mu_i\}, \{\rho_{ij}\}\}$ is a set of auxiliary parameters to determine later, and the functions G_i and J_{ij} are such that

$$\begin{aligned} T_i'(G_i(x)) - \frac{G_i(x)}{x} &= 0, \\ V_{ij}'(J_{ij}(x)) - 2x J_{ij}(x) &= 0, \end{aligned} \tag{3}$$

where $U'(x) = dU(x)/dx$. It is useful to write Hamiltonian (2) in the form

$$\tilde{H}(\{\alpha\}) = H_{\text{ho}}(\{\alpha\}) + B(\{\alpha\}), \tag{4}$$

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where $H_{\rm ho}$ is the harmonic oscillator part and B is a function obtained by subtracting the harmonic oscillator contributions from (2). An eigenvalue of (2) is given by

$$\tilde{E}(\{\alpha\}) = E_{\rm ho}(\{\alpha\}) + B(\{\alpha\}), \tag{5}$$

where $E_{\rm ho}$ is an eigenvalue of $H_{\rm ho}$. A procedure in [6, 11] explains how to compute $E_{\rm ho}$ but an example will be given below. An eigenvalue $\tilde{E}$ also depends on the set of parameters $\{\alpha\} = \{\{\mu_i\}, \{\rho_{ij}\}\}$. The principle of the method is to search for the set of parameters $\{\alpha_0\} = \{\{\mu_{i0}\}, \{\rho_{ij0}\}\}$ such that

$$\left.\frac{\partial \tilde{E}}{\partial \mu_i}\right|_{\{\alpha_0\}} = \left.\frac{\partial \tilde{E}}{\partial \rho_{ij}}\right|_{\{\alpha_0\}} = 0 \quad \forall\ i, j. \tag{6}$$

Equations (6) can be easily implemented and solutions $\{\alpha_0\}$ are easily found since we only need to find an extremum [6]. After solving (6), we obtain the desired approximate energy by substituting the set $\{\alpha_0\}$ back to (5), $\tilde{E}(\{\alpha_0\}) = \tilde{E}_0$.

In the case of identical particles, it has been showed [4, 5] that we can equivalently find the eigenvalue (5) by using a set of three compact equations

$$\tilde{E}_0 = N\,T(p_0) + C_N^2\,V(\rho_0), \tag{7a}$$

$$N\,T'(p_0)\,p_0 = C_N^2\,V'(\rho_0)\,\rho_0, \tag{7b}$$

$$Q(N) = \sqrt{C_N^2}\,p_0\,\rho_0, \tag{7c}$$

where $p_0^2 = \langle \boldsymbol{p}_i^2 \rangle$ and $\rho_0^2 = \langle \boldsymbol{r}_{ij}^2 \rangle \ \ \forall\ i, j$. The mean values are taken with an eigenstate of the auxiliary Hamiltonian corresponding to the global quantum number $Q(N)$ for the set $\{\alpha_0\}$ insuring the constraints (6). The eigenstate is also completely (anti)symmetric for the exchange between particles.

$$Q(N) = \begin{cases} \sum\limits_{i=1}^{N-1} \left(2n_i + l_i + \frac{D}{2}\right) & \text{if } D \geq 2 \\ \\ \sum\limits_{i=1}^{N-1} \left(n_i + \frac{1}{2}\right) & \text{if } D = 1 \end{cases}, \tag{8}$$

where the quantum numbers n_i (l_i) are associated with the internal variables. Some values of $Q(N)$ for the bosonic and fermionic ground states are given in [5, 6]. In previous papers [4, 5], the variable $r_0^2 = N^2 \left\langle (\boldsymbol{r}_i - \boldsymbol{R})^2 \right\rangle$, where $\boldsymbol{R}$ is the CM position, was used instead of ρ_0 because one-body and two-body potentials are treated at the same time.

Equations (7) can also be easily implemented and solved. There are good reasons to prefer the compact equations (7) over the "extremization" equations (6). First, the quantities p_0 and ρ_0 give direct access to more interesting expectation values than $\{\alpha_0\}$. Secondly, these equations have a nice semiclassical interpretation as explained in [4]. Thirdly, it is possible to improve the ET with the dominantly orbital state method starting from these equations [12]. Unfortunately, such equations are only known for identical particles. In the following section, we will present the compact equations for a system composed of two different sets of N_a and N_b identical particles.

II. $N_a + N_b$ SYSTEMS

Let us specify the auxiliary Hamiltonian (2) for this system. The harmonic oscillator Hamiltonian for a system of N_a particles of type a and N_b particles of type b is given by

$$H_{\rm ho} = \sum_{i=1}^{N_a} \frac{\boldsymbol{p}_i^2}{2\mu_a} + \sum_{j=1}^{N_b} \frac{\boldsymbol{p}_j^2}{2\mu_b} + \sum_{i<i'=2}^{N_a} \rho_{aa} \boldsymbol{r}_{ii'}^2 + \sum_{j<j'=2}^{N_b} \rho_{bb} \boldsymbol{r}_{jj'}^2 + \sum_{i=1}^{N_a} \sum_{j=1}^{N_b} \rho_{ab} \boldsymbol{r}_{ij}^2. \tag{9}$$

In the following, letters i (j) are reserved for particles of type a (b). As explained in [6, 7], it is useful to write (9) in the form

$$H_{\rm ho} = H_a + H_b + H_{\rm CM} \qquad \text{with} \tag{10a}$$

$$H_a = \sum_{i=1}^{N_a} \frac{\boldsymbol{p}_i^2}{2\mu_a} - \frac{\boldsymbol{P}_a^2}{2M_a} + \sum_{i<i'=2}^{N_a} \left(\rho_{aa} + \frac{N_b}{N_a}\rho_{ab}\right) \boldsymbol{r}_{ii'}^2, \tag{10b}$$

$$H_b = \sum_{j=1}^{N_b} \frac{\boldsymbol{p}_j^2}{2\mu_b} - \frac{\boldsymbol{P}_b^2}{2M_b} + \sum_{j<j'=2}^{N_b} \left(\rho_{bb} + \frac{N_a}{N_b}\rho_{ab}\right) \boldsymbol{r}_{jj'}^2, \tag{10c}$$

$$H_{\mathrm{CM}} = \frac{\boldsymbol{p}^2}{2\mu} + N_a N_b \rho_{ab} \boldsymbol{r}^2, \tag{10d}$$

where $\boldsymbol{P}_\alpha$ and M_α are the total momentum and mass for the set $\alpha = \{a, b\}$, $\mu = \frac{M_a M_b}{M_a + M_b}$ is a reduced mass, and $\boldsymbol{p} = \frac{M_b \boldsymbol{P}_a - M_a \boldsymbol{P}_b}{M_a + M_b}$ and $\boldsymbol{r} = \boldsymbol{R}_a - \boldsymbol{R}_b$ are the relative momentum and position between the CM of the two sets, respectively. The three parts of (10) are entirely decoupled since (10b) and (10c) depends on the internal coordinates of their respective set, and (10d) on the relative coordinates between the two CM.

Then, an eigenvalue E_{ho} is easily obtained since (10) is composed of three decoupled parts [6]

$$E_{\mathrm{ho}} = Q(N_a)\sqrt{\frac{2}{\mu_a}(N_a\rho_{aa} + N_b\rho_{ab})} + Q(N_b)\sqrt{\frac{2}{\mu_b}(N_b\rho_{bb} + N_a\rho_{ab})} + Q(2)\sqrt{\frac{2}{\mu}N_a N_b \rho_{ab}}. \tag{11}$$

To be complete, the expression of the function $B(\{\alpha\})$ is given by

$$\begin{aligned} B = {} & N_a \left[T_a(G_a(\mu_a)) - \frac{G_a^2(\mu_a)}{2\mu_a}\right] + C_{N_a}^2 \left[V_{aa}(J_{aa}(\rho_{aa})) - \rho_{aa} J_{aa}^2(\rho_{aa})\right] \\ & + N_b \left[T_b(G_b(\mu_b)) - \frac{G_b^2(\mu_b)}{2\mu_b}\right] + C_{N_b}^2 \left[V_{bb}(J_{bb}(\rho_{bb})) - \rho_{bb} J_{bb}^2(\rho_{bb})\right] \\ & + N_a N_b \left[V_{ab}(J_{ab}(\rho_{ab})) - \rho_{ab} J_{ab}^2(\rho_{ab})\right]. \end{aligned} \tag{12}$$

When combining (10) and (12), we can see that our auxiliary Hamiltonian (2) is also composed of three distinct parts: one for the particles of type a, another for the particles of type b and a last one for the relative motion between the two sets.

The compact equations can then be established in a similar way as done for identical particles [13]. First, we apply the Hellmann-Feynman theorem [14] on Hamiltonian (2) to evaluate extremization conditions (6). By using definitions (3) we get the following results

$$\begin{aligned} & G_a^2(\mu_{a0}) = p_a^2 + \tfrac{P_0^2}{N_a^2} = {p'_a}^2, \\ & G_b^2(\mu_{b0}) = p_b^2 + \tfrac{P_0^2}{N_b^2} = {p'_b}^2, \\ & J_{aa}^2(\rho_{aa0}) = r_{aa}^2, \\ & J_{bb}^2(\rho_{bb0}) = r_{bb}^2, \\ & J_{ab}^2(\rho_{ab0}) = \tfrac{N_a - 1}{2N_a} r_{aa}^2 + \tfrac{N_b - 1}{2N_b} r_{bb}^2 + R_0^2 = {r'_0}^2, \end{aligned} \tag{13}$$

where we have defined the six physical parameters

$$\begin{aligned} & p_a^2 = \left\langle \boldsymbol{p}_i^2 - \tfrac{\boldsymbol{P}_a^2}{N_a^2} \right\rangle \text{ and } p_b^2 = \left\langle \boldsymbol{p}_j^2 - \tfrac{\boldsymbol{P}_b^2}{N_b^2} \right\rangle, \\ & r_{aa}^2 = \left\langle \boldsymbol{r}_{ii'}^2 \right\rangle \text{ and } r_{bb}^2 = \left\langle \boldsymbol{r}_{jj'}^2 \right\rangle, \\ & P_0^2 = \left\langle \boldsymbol{p}^2 \right\rangle \text{ and } R_0^2 = \left\langle \boldsymbol{r}^2 \right\rangle. \end{aligned} \tag{14}$$

The mean values are taken with an eigenstate of the auxiliary Hamiltonian corresponding to the quantum numbers $Q(N_a)$, $Q(N_b)$ and $Q(2)$ for the set $\{\alpha_0\}$ insuring the constraints (6). The eigenstate is also completely (anti)symmetric for the exchange between the N_a or the N_b particles.

Then, by evaluating $\tilde{E}_0 = \left\langle \tilde{H}(\{\alpha_0\}) \right\rangle$ and using results (13), we obtain the following equation for the energy

$$\tilde{E}_0 = N_a T_a\left(p'_a\right) + N_b T_b\left(p'_b\right) + C_{N_a}^2 V_{aa}\left(r_{aa}\right) + C_{N_b}^2 V_{bb}\left(r_{bb}\right) + N_a N_b V_{ab}\left(r'_0\right) \tag{15}$$

It is interesting to look at the meaning of the linear combinations p'_a, p'_b and r'_0 since they appear in (15). As shown in [6], we can derive a similar equation for the energy by using the form (9), instead of (10), for the harmonic oscillator. By comparing, one can identify ${p'_a}^2 = \langle \boldsymbol{p}_i^2 \rangle$, ${p'_b}^2 = \langle \boldsymbol{p}_j^2 \rangle$ and ${r'_0}^2 = \langle \boldsymbol{r}_{ij}^2 \rangle$.

In order to find these parameters, we need 6 additional equations. We can find three of them by applying the virial theorem [6] separately on each of the three parts of the auxiliary Hamiltonian. One gets

$$N_a T'_a(p'_a) \frac{1}{p'_a} p_a^2 = C_{N_a}^2 r_{aa} V'_{aa}(r_{aa}) + \frac{N_b}{N_a} C_{N_a}^2 V'_{ab}(r'_0) \frac{1}{r'_0} r_{aa}^2, \tag{16a}$$

$$N_b T'_b(p'_b) \frac{1}{p'_b} p_b^2 = C_{N_b}^2 r_{bb} V'_{bb}(r_{bb}) + \frac{N_a}{N_b} C_{N_b}^2 V'_{ab}(r'_0) \frac{1}{r'_0} r_{bb}^2, \tag{16b}$$

$$T'_a(p'_a) \frac{1}{p'_a} \frac{P_0^2}{N_a} + T'_b(p'_b) \frac{1}{p'_b} \frac{P_0^2}{N_b} = N_a N_b V'_{ab}(r'_0) \frac{1}{r'_0} R_0^2. \tag{16c}$$

Finally, we obtain three last equations by using the exact eigenvalue (11) of the harmonic oscillator and comparing it to $\langle H_{\rm ho}\{\alpha_0\}\rangle$. Thanks to (10), the comparison is done in a similar way as in [13] and one gets

$$Q(N_a) = \sqrt{C_{N_a}^2}\, p_a r_{aa}, \tag{17a}$$

$$Q(N_b) = \sqrt{C_{N_b}^2}\, p_b r_{bb}, \tag{17b}$$

$$Q(2) = P_0 R_0. \tag{17c}$$

Equations (16) and (17) form a set of six equations which, combined with (15), allow us to compute the approximate eigenvalue $\tilde{E}_0$ and form the ET compact equations for a system of $N_a + N_b$ particles. We can note that the three equations (16) can be derived by minimizing (15) with respect to r_{aa}, r_{bb} and R_0, and using (17).

Equations (15)-(17) are more complicated than equations (7). But, by comparing the two sets, it is possible to find an interpretation for equations (15)-(17). Equation (15) is obviously the energy computed in terms of the mean momentums and relative distances. Equations (16) are the equations of motion determining these mean quantities, and equations (17) are the semiclassical quantifications of the various orbital and radial motions. These equations make clear what are the relevant quantities appearing in a quantum system containing two different sets of identical particles. It is worth recalling that solutions obtained by the ET are full quantum ones with eigenfunctions associated [6, 11] and that observables can be computed [9].

As a first check for these equations, we need to retrieve the three equations (7) when considering all particles identical. In this case $T_a = T_b$ and $V_{aa} = V_{bb} = V_{ab}$, and we must impose the following symmetries

$$\begin{aligned} \left\langle \boldsymbol{p}_i^2 \right\rangle &= \left\langle \boldsymbol{p}_j^2 \right\rangle, \quad \forall\ i, j, \\ \left\langle \boldsymbol{r}_{ii'}^2 \right\rangle &= \left\langle \boldsymbol{r}_{jj'}^2 \right\rangle = \left\langle \boldsymbol{r}_{ij}^2 \right\rangle, \quad \forall\ i, i', j, j'. \end{aligned} \tag{18}$$

From the definitions of our 6 parameters, we conclude

$$\begin{aligned} p'_a &= p'_b = p_0, \\ r_{aa} &= r_{bb} = r'_0 = \rho_0, \end{aligned} \tag{19}$$

where p_0 and ρ_0 are defined as before in (7). Then, we easily see that equation (15) reduces to (7a) with $N = N_a + N_b$. It is a matter of algebra to show that the sum of the three equations (16)

$$N_a T'_a(p'_a) p'_a + N_b T'_b(p'_b) p'_b = C_{N_a}^2 V'_{aa}(r_{aa}) r_{aa} + C_{N_b}^2 V'_{bb}(r_{bb}) r_{bb} + N_a N_b V'_{ab}(r'_0) r'_0, \tag{20}$$

reduces to (7b). When all the particles are identical, it is not relevant to separate the energy on several subsets. We notice that $Q(N_a) + Q(N_b) + Q(2) = Q(N_a + N_b)$. This is a hint that the sum of the three equations (17) must reduce to (7c), but the proof is more subtle. Thanks to the symmetries (18) and (19), one can express R_0 in terms of ρ_0, and p_a, p_b and P_0 in terms p_0. Then, simple calculations show that (17) reduces to (7c). Finally, all equations (7) are recovered. Note that (19) also implies symmetries on the auxiliary parameters, $\mu_a = \mu_b$ and $\rho_{aa} = \rho_{bb} = \rho_{ab}$, which is also expected as explained in [6].

As a second test, we have substituted the harmonic oscillator Hamiltonian (9) into our seven equations. Then, it is a matter of algebra to find the exact solution (11).

III. $N_a = 1$ OR/AND $N_b = 1$

The seven equations (15), (16) and (17) were computed for a system with $N_a + N_b$ particles. It is interesting to look at what happens when only one particle is present in a set. For example, let's look at the case $N_b = 1$. Then, all the terms in $C^2_{N_b}$ and $Q(N_b)$ vanish. Equation (17b) becomes trivial and (16b) leads to $p_b = 0$. As $p_b = 0$, we also have $p'_b = P_0$. At the end, we are left with a system of 5 equations

$$\tilde{E}_0 = N_a T_a\left(p'_a\right) + T_b\left(P_0\right) + C^2_{N_a} V_{aa}\left(r_{aa}\right) + N_a V_{ab}\left(r'_0\right), \tag{21a}$$

$$N_a T'_a(p'_a)\frac{1}{p'_a}p_a^2 = C^2_{N_a} r_{aa} V'_{aa}(r_{aa}) + \frac{1}{N_a} C^2_{N_a} V'_{ab}(r'_0)\frac{1}{r'_0} r_{aa}^2, \tag{21b}$$

$$T'_a(p'_a)\frac{1}{p'_a}\frac{P_0^2}{N_a} + T'_b(P_0)P_0 = N_a V'_{ab}(r'_0)\frac{1}{r'_0} R_0^2, \tag{21c}$$

$$Q(N_a) = \sqrt{C^2_{N_a}}\, p_a r_{aa}, \tag{21d}$$

$$Q(2) = P_0 R_0, \tag{21e}$$

where our four parameters are now defined as $p_a^2 = \left\langle \boldsymbol{p}_i^2 - \frac{\boldsymbol{P}_a^2}{N_a^2} \right\rangle$, $P_0^2 = \left\langle \left(\frac{\mu_b \boldsymbol{P}_a - M_a \boldsymbol{p}_b}{M_a + \mu_b} \right)^2 \right\rangle$, $\boldsymbol{r}_{aa}^2 = \left\langle \boldsymbol{r}_{ii'}^2 \right\rangle$ and $R_0^2 = \left\langle (\boldsymbol{R}_a - \boldsymbol{r}_b)^2 \right\rangle$, and we have ${p'_a}^2 = p_a^2 + \frac{P_0^2}{N_a^2}$ and ${r'_0}^2 = \frac{N_a - 1}{2N_a} r_{aa}^2 + R_0^2$. The five equations (21) can also be found from scratch with the above explained procedure.

Another special case is when $N_a = N_b = 1$, that is we have a two-body system. We then have similar simplifications as in the previous case and we obtain the equations of the envelope theory at $N = 2$, which are a generalization of the results obtained in [4, 15]

$$\tilde{E}_0 = T_a(P_0) + T_b(P_0) + V_{ab}(R_0), \tag{22a}$$

$$T'_a(P_0)P_0 + T'_b(P_0)P_0 = V'_{ab}(R_0)R_0, \tag{22b}$$

$$Q(2) = P_0 R_0, \tag{22c}$$

where $P_0^2 = \left\langle \left(\frac{\mu_b \boldsymbol{p}_a - \mu_a \boldsymbol{p}_b}{\mu_a + \mu_b} \right)^2 \right\rangle$ and $R_0^2 = \left\langle (\boldsymbol{r}_a - \boldsymbol{r}_b)^2 \right\rangle$.

IV. CONCLUDING REMARKS

We were able to build the 7 compact equations of the envelope theory for a system of $N_a + N_b$ particles. These equations reduce to the three usual ones when considering identical particles. We also presented the special cases when $N_b = 1$ or/and $N_a = 1$. The 5 equations for a system of $N_a + 1$ particles are currently used in order to improve the method and will be the subject of a future paper [16]. We have verified that those equations give the same results found with the extremization equations in [6].

Acknowledgments

L.C. would thank the Fonds de la Recherche Scientifique - FNRS for the financial support. This work was also supported under Grant Number 4.45.10.08.

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