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POINT TRANSFORMATION IN A MANY-PARTICLE SYSTEM

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ABSTRACT: In this paper we modify the many-particle point transforms previously developed by N.M. Witriol in such a way that the transformation varies from the identity transformation - one isolated body - to the *N*-bodies interacting as the interparticle separations fall within an arbitrary chosen cutoff distance. The method is used to provide Hamiltonians for strongly interacting particles that are equivalent to the usual Hamiltonians.

1. INTRODUCTION

The method of point transformation, as developed by F.M. Eger and E.P. Gross[3-6], is basically a classical canonical transformation of the variables of the system and it then quantizes these transformed variables. They began to explore the use of this method in many-particle theory, with the main purpose of obtaining Hamiltonians free of the difficulties encountered in dealing with strongly interacting particles. Using this method, Eger and Gross have assumed that for a sufficiently dilute system the equivalent many-

body Hamiltonians are the sum over all pairs of two-body Hamiltonians. When this pairwise point transformation method is applied to deduce the main properties of low temperature quantum liquids, such as the ground state energy and the low-level excitations of the hard-core Bose liquid[5], they are found to agree with the low-density results of Lee, Huang, and Yang[7]. Similarly, when the method in this pairwise limit, as developed by Eger and Gross, is applied to the many-body hard-core Fermi system[8], the ground state energy and Landau parameters are in agreement with those of Abrikosov and Khalatnikov[10]. In essence, in these methods approximations are rigorously valid only in the limit of low-density (smallness of the ratio $c\rho^3$, where ρ is the density and c is the radius of the hard-core potential). For physical systems of interest, such as liquid ^{3}He, ^{4}He, and nuclear matter, the conditions for the validity of these approximations are not actually satisfied.

Recently, N.M. Witriol[1,2] has extended the method of point transform to the consideration of the truly many-particle terms of many-particle systems. Witriol's methods have been based on the previous point transformation method developed by Eger and Gross[3-6]. In his first paper[1], Witriol developed an interacting particle cluster method for transforming the many-body hard-core Hamiltonian into a less singular and equivalent Hamiltonian. The transformation is taken to be regional – one free particle, two interacting particles, three interacting particles, ... N-interacting particles, as desired – and continuous in the $3N$-dimensional configuration space. The cluster transformation functions were defined in a manner such that each N-particle cluster would shrink about its center of mass; the shrinkage factor depending on the smallest interparticle separation. Mathematically, these transformation functions depend only on the two-body smallest distance. For large clusters – more than two-body interactions – the form of the transformations leads to laborius mathematical computations as a result of the continuous and cutoff conditions on the cluster formalism. In his second attempt[2], Witriol removed the cutoff terms in the transformation. Essentially, it is an N-body cluster where the cutoff distance of the new transformation is taken to be ∞ throughout the configuration space. To facilitate the calculation of this hard-core N-particle term, the transformation function is restricted to being also regional as in his previous work, regions being determined by the smallest interparticle separation; that is to say, the transformation function is restricted to depend only on the smallest distance between the particles. Moreover, because of the very long range of the transformation function used, the resulting Hamiltonian does not approach the free particle Hamiltonian for large values of the interparticle separation, and the original and transformed wave function differs asymptotically for large r, which is of course somewhat

inconvenient in discussing scattering problems.

In this article we suggest a new transformation function without using the cluster formalism introduced by Witriol[1,2]. In the resulting configuration space the system is also shrunk around its center of mass with the same purpose of reducing the effects of the short-range, strongly repulsive or hard-core potential, but with a cutoff conditions in such a way that the transformation varies from the identity transformation – one particle isolated – to the N-bodies interacting, as the interparticle separations fall within an arbitrary chosen cutoff distance. In other words, when the mean interparticle separation is much larger than a certain distance, the probability of a configuration with higher order of particles within this distance of each other is negligible. For large interacting terms the expansion technique caused by this transformation gives rise to less mathematical computation than that caused by the functional form of the transformation suggested by Witriol.

In sec. 2 we define a transformation of coordinates and construct the corresponding family of transformation functions on the ground of continuity, one-to-one and invariance conditions. In sec. 3 the transformation is used for transforming the many-body hard-core Hamiltonian into an equivalent, "well behaved" set of hermitian Hamiltonians. We note how, in the limit of the two-particle interaction term, the resulting set of point transformation approximates the set of pairwise point transformation developed by Eger and Gross[3-6] and how it emerges in an elementary and unambiguous way. In the final section we give a discussion and compile the general remarks of the present work.

2. DEFINITION OF THE TRANSFORMATION

Let us start by defining the transformation which is essentially a transformation of coordinates. Notationally, Latin indices refer to particle indices (from 1 to N), Greek indices refer to cartesian space coordinates (from 1 to 3), capital letters refer to original variables, and small letters to the transformed variables. The original coordinates $X_{i\alpha}$ are related to the transformed coordinates $x_{i\alpha}$ according to the following transformation:

$$X_{i\alpha} - \overline{X}_\alpha = \phi(\ldots x_{i\alpha} \ldots)(x_{i\alpha} - \overline{x}_\alpha) , \tag{2.1}$$

where the transformation function ϕ is an arbitrary real function of the position of the particles; $\overline{X}_\alpha$ and $\overline{x}_\alpha$ represent the center of mass coordinate of the N-body system in each configuration space, that is

$$\overline{X}_\alpha = (1/N) \sum_{i=1}^{N} X_{i\alpha} \ . \tag{2.2}$$

The center of mass is thus chosen as the reference point of the transformation. If the center of mass motion is not altered, then $\overline{X}_\alpha = \overline{x}_\alpha$; and it immediately follows from eq. (2.1) that the transformation may be written in the form

$$X_{i\alpha} = \phi\, x_{i\alpha} + (1-\phi)\overline{x}_\alpha \ . \tag{2.3}$$

Let us now examine our function ϕ in detail. If the system is invariant under simultaneous rotation of the coordinates of the system, ϕ must be a symmetric function of the difference of the coordinates. Since our problem is to make "soft" the "hard-core", the range of ϕ must be considerably greater than the diameter c of this core. Notice that we only need to specify the function, which, of course, plays an important role in the theory for making strong statements about the behaviour of the dynamical variables, the coordinates and momenta, depending upon the form we may choose for this function. The transformation shall be chosen to shrink the system, reducing or eliminating in this way - depending of this choice - the strong short range potential. We wish to consider next how the function ϕ can be built from general considerations about the interactions of the particles. First of all, if ϕ must include the identity transformation, then $\phi \to 1$ as the distance R_{ij} between any two particles i and j is larger than certain distance b, taken to be larger than the radius of the hard-core, c, to guarantee the one-to-oneness of the transformation, so

$$R_{ij} = r_{ij} \qquad \text{for } (R_{ij}, r_{ij}) > b \ , \tag{2.4}$$

where r_{ij} is the interparticle separation in the transformed configuration space. The transformation is then healed in a distance b which acts as a cutoff parameter and as the range of the interaction created by this transformation. Our purpose is to modify the direct potential, which in this case is a hard-core type; since under the transformation (eq. 2.3), the potential becomes

$$V'(R) = V\,[R(r)] = V\,[\phi(r)] \ , \tag{2.5}$$

and, since in the original space the potential is

$$V'(R) = \infty \ , \ R < c$$
$$V'(R) = 0 \ , \ R > c \qquad (2.6)$$

then the class of functions

$$\phi = 1 + f \ , \qquad (2.7)$$

where

$$f \to c/r \quad \text{when} \quad r \to 0 \qquad (2.8)$$

and c is equal to the core diameter, removes completely the hard-core, that is, from eq. (2.5), we obtain $V(r) = 0$ over all space. We note also, from the condition on ϕ established above, that

$$f \to 0 \quad \text{when each} \quad r_{ij} \to b \ . \qquad (2.9)$$

Then the characteristics of the problem are thrown now onto f.

If the two-body encounters are dominant in the interaction, we write f as

$$f(r) = [c/(r + \epsilon)]\, g(r)$$

so, for the two-body interacting terms we have:

$$f_{\text{two-body}} = \sum_{\substack{i,j=1 \\ i<j}}^{N} [c/(r_{ij} + \epsilon)]\, g(r_{ij}) \ . \qquad (2.10)$$

We may imagine $\epsilon > 0$ and pass to the limit $\epsilon \to 0$ after all phase shifts, matrix elements, etc., have been evaluated. Clearly, the function g is chosen such that

$$g(r_{ij}) \to 1 \quad , \quad r_{ij} \to 0$$
$$g(r_{ij}) \to 0 \quad , \quad r_{ij} \to b \qquad (2.11)$$

In this case the probability of a configuration with more than two particles within a distance b is negligible.

To consider the third order interaction terms we should take into account the continuous transition between these terms and the two-body terms, when the probability that a third body were correlated to other two bodies which are certainly correlated, is small. We shall assume that they can be built up as a product of pair terms, similar to the form that has been proposed for the three-atom correlation function in the Born-Green theory of liquids[11]. Thus, we write the three-body term:

$$\sum_{\substack{i,j,k=1 \\ i<j<j}}^{N} \gamma_{ijk}\, g(r_{ij})\, g(r_{jk})(1 - g_{ik}) \ , \qquad (2.12)$$

where γ_{ijk} depends only on the smallest interparticle separation between the particles i, j, k. That is, it has the form

$$\gamma_{ijk} = c/(r_{ij} + \epsilon) \ \text{ if } \ r_{ij} < r_{ik} < r_{jk} \ , \qquad (2.13)$$

or

$$\gamma_{i_1 i_2 i_3} = (\tau_3)^{-1} \sum_{\substack{c,d=1 \\ c<d \\ i_a i_b \neq i_c i_d}}^{3} \prod_{\substack{a,b=1 \\ a<b}}^{3} \theta(r_{i_a i_b} - r_{i_c i_d}) \frac{c}{r_{i_c i_d} + \epsilon} \ , \qquad (2.13b)$$

where

$$\tau_3 = \sum_{\substack{c,d=1 \\ c<d \\ i_a i_b \neq i_c i_d}}^{3} \prod_{\substack{a,b=1 \\ a<b}}^{3} \theta(r_{i_a i_b} - r_{i_c i_d}) \ , \qquad (2.13c)$$

and $i_a i_b$ means that $r_{i_a i_b}$ and $r_{i_c i_d}$ are not the same interparticle spacing, and the product over the θ is such that

$$\theta\,(r_{i_a i_b} - r_{i_c i_d}) = \begin{cases} 0\,, & r_{i_a i_b} < r_{i_c i_d} \\ 1\,, & r_{i_a i_b} \geqslant r_{i_c i_d} \end{cases} \tag{2.14}$$

If the fourth order interaction terms are considered, we also assume that they can be built up as a product of pair terms, then the four body term is as follows:

$$\sum_{\substack{i,\,j,\,k,\,l\,=\,1 \\ i<j<k<1}}^{N} \gamma_{ijkl}\, g_{ij}\, g_{jk}\, g_{kl}\, g_{jl}\,(1-g_{ik})(1-g_{il}) \tag{2.15}$$

where γ_{ijkl} is defined as above, depending on the smallest interparticle spacing between the particles i, j, k, l.

We illustrate the general features of the transformation by showing diagrammatically the first lower order terms:

1 - particle isolated (i): $(R_{ij}\,,\, r_{ij}) > b$ all $j \neq i$, $1 \leqslant j \leqslant N$

$i\bullet$ $\qquad\qquad$ $\phi_i \to 1$

2 - particles interacting (ij): $(R_{ik}\,,\, R_{jk}\,;\, r_{ik}\, r_{jk}) > b$

$(R_{ij}\,,\, r_{ij}) \leqslant b$, all $k \neq i, j$, $1 \leqslant k \leqslant N$

$i\bullet\!\!-\!\!-\!\!-\!\!-\!\!-\!\!-\!\!-\!\!-\!\!\bullet j$ $\qquad\qquad$ $\phi_{ij} \to 1 + [c/(r_{ij} + \epsilon)]\; g(r_{ij})$

3 - particles interacting (ijk):

$(R_{il}\,,\, R_{jl}\,,\, R_{kl}\,;\, r_{il}\,,\, r_{jl}\,,\, r_{kl}) > b$ all $l \neq i, j, k$. $1 \leqslant l \leqslant N$

which in the case $(R_{ik}, R_{jk}, R_{ij}; r_{ik}, r_{jk}, r_{ij}) \leq b$, we have

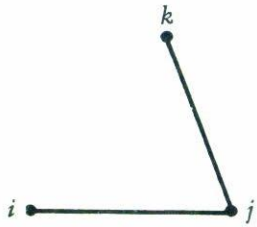
$$\phi_{ijk} = [1 + c/(r_{ij} + \epsilon)]\, g(r_{ij}) +$$

$$[c/(r_{jk} + \epsilon)]\, g(r_{jk}) + [c/(r_{ik} + \epsilon)]\, g(r_{ik}) +$$

$$\gamma_{ijk} \left\{ g(r_{ij}) g(r_{jk}) [1 - g(r_{ik})] + \right.$$

$$\left. g(r_{ij}) g(r_{ik}) [1 - g(r_{jk})] + g(r_{jk}) g(r_{ik}) [1 - g(r_{ij})] \right\} .$$

For the case $(R_{ij}, R_{jk}; r_{ij}, r_{jk}) \leq b$; $(R_{ik}, r_{ik}) > b$, then



$$\phi_{ijk} \to 1 + [c/(r_{ij} + \epsilon)]\, g(r_{ij}) +$$

$$[c/(r_{jk} + \epsilon)]\, g(r_{jk}) + \gamma_{ijk}\, g(r_{ij}) g(r_{jk})$$

and so on. We easily note that the form chosen for ϕ_{ijk} is in concordance with the continuity conditions of the transformation.

3. THE HAMILTONIAN

Clearly, the relationship between the transformed momenta $p_{i\alpha}$ and the original momenta $P_{j\beta}$, according to the definition of our point transformation, eq. (2.3), and due to the hermiticity conditions on this operator, is

$$P_{i\alpha} = \tfrac{1}{2} \sum_{j=1}^{N} \sum_{\beta=1}^{3} \left[\frac{\partial x_{j\beta}}{\partial X_{i\alpha}} p_{j\beta} + p_{j\beta} \frac{\partial x_{j\beta}}{\partial X_{i\alpha}} \right] \tag{3.1}$$

where $p_{j\beta} = -i\hbar\, \partial/\partial x_{j\beta}$. In checking that X and P obey the correct commutation rules, one needs the theorems[12]:

$$\frac{\partial \log A}{\partial x_{i\alpha}} = \sum_{j,\beta} \frac{\partial}{\partial X_{j\beta}} \left[\frac{\partial X_{j\beta}}{\partial x_{i\alpha}} \right]$$

$$\sum_{j,\beta} \frac{\partial}{\partial x_{j\beta}} \left[A \frac{\partial x_{j\beta}}{\partial X_{i\alpha}} \right] = 0 , \tag{3.2}$$

where A is the $3N$ th-order Jacobian $\left| \frac{\partial X_{i\alpha}}{\partial x_{i\beta}} \right|$ related to the 3N th-order Jacobian $B = \left| \frac{\partial x_{i\alpha}}{\partial X_{j\beta}} \right|$ of the inverse transformation by the relation

$$A \cdot B = 1 . \tag{3.3}$$

This allows us to write $P_{i\alpha}$ in the alternative form

$$P_{i\alpha} = \sum_{j=1}^{N} \sum_{\beta=1}^{3} \frac{\partial x_{j\beta}}{\partial X_{i\alpha}} \left[p_{j\beta} + \frac{i\hbar}{2} \frac{\partial \log A}{\partial x_{j\beta}} \right]$$

$$= \sum_{j=1}^{N} \sum_{\beta=1}^{3} \left[p_{j\beta} - \frac{i\hbar}{2} \frac{\partial \log A}{\partial x_{j\beta}} \right] \frac{\partial x_{j\beta}}{\partial X_{i\alpha}} . \tag{3.4}$$

By means of this transformation the original Hamiltonian

$$H(\boldsymbol{R}, \boldsymbol{P}) = \sum_{i=1}^{N} \sum_{\alpha=1}^{3} p_{i\alpha}^2 + V(\boldsymbol{R}, \boldsymbol{P}) \tag{3.5}$$

(where $\boldsymbol{R}, \boldsymbol{P}, \boldsymbol{r}, \boldsymbol{p}$, represent their respective set of $3N$ variables $\boldsymbol{R}_i, \boldsymbol{P}_i, \boldsymbol{r}_i, \boldsymbol{p}_i$) is transformed into itself according to

$$H'(\boldsymbol{r}, \boldsymbol{p}) = H\left[\boldsymbol{R}(\boldsymbol{r}), \boldsymbol{P}(\boldsymbol{r}, \boldsymbol{p})\right] = \sum_{i,j=1}^{N} \sum_{\alpha,\beta=1}^{3} p_{i\alpha} \mathfrak{L}_{i\alpha j\beta} p_{j\beta} +$$

$$V(\boldsymbol{r}, \boldsymbol{p}) + W(\boldsymbol{r}) , \tag{3.6}$$

where

$$\mathcal{L}_{i\alpha j\beta} = \sum_{l=1}^{N} \sum_{\tau=1}^{3} \frac{\partial x_{i\alpha}}{\partial X_{l\tau}} \frac{\partial x_{j\beta}}{\partial X_{l\tau}} ,$$

and

$$W(r) = \sum_{i,j=1}^{N} \sum_{\alpha,\beta=1}^{3} \left[\tfrac{1}{2} \mathcal{L}_{i\alpha j\beta} \frac{\partial \log A}{\partial x_{i\alpha}} \frac{\partial \log A}{\partial x_{j\beta}} + \tfrac{1}{2} \frac{\partial}{\partial x_{j\alpha}} \left(\mathcal{L}_{i\alpha j\beta} \frac{\partial \log A}{\partial x_{j\beta}} \right) \right] \tag{3.7}$$

In order to ensure that the Schrödinger's equation in both configuration spaces leads to the same eigenvalue E, the corresponding wave function may be related by

$$\Psi_E \left[\boldsymbol{R}(r) \right] = \boldsymbol{B}^{1/2}(r)\, \Psi'(r) \tag{3.8}$$

or, by the eq. (3.3)

$$\Psi_E(\boldsymbol{R}) = A^{-1/2}(\boldsymbol{R})\, \Psi'_E \left[\boldsymbol{r}(\boldsymbol{R}) \right] . \tag{3.9}$$

The Jacobians ensure the preservation of the normalization of wave functions as may be easily checked.

Let us evaluate now $\partial x_{i\alpha}/\partial X_{j\beta}$. By differentiating eq. (2.3) with respect to $X_{l\tau}$ we find

$$\delta_{il}\delta_{\alpha\tau} = \sum_{k=1}^{N} \sum_{\lambda=1}^{3} \frac{\partial \phi}{\partial x_{k\lambda}} \frac{\partial x_{k\lambda}}{X_{l\tau}} (x_{i\alpha} - \overline{x}_\alpha) + \phi \frac{\partial x_{i\alpha}}{\partial X_{l\tau}} +$$

$$\frac{1-\phi}{N} \sum_{k=1}^{N} \frac{\partial x_{k\lambda}}{\partial X_{l\tau}} , \tag{3.10}$$

but by the definition of $\overline{x}_\alpha = \overline{X}_\alpha = \sum_{k=1}^{N} x_{k\alpha}$ it follows immediately that

$$\sum_{k=1}^{N} \frac{\partial x_{k\alpha}}{\partial X_{l\tau}} = \sum_{k=1}^{N} \frac{\partial X_{k\alpha}}{\partial x_{l\tau}} = \delta_{\alpha\tau} ,$$

so that eq. (3.10) leads to

$$[\delta_{il} - (1-\phi)/N]\,\delta_{a\tau} = \sum_{k=1}^{N}\sum_{\lambda=1}^{3}\frac{\partial\phi}{\partial x_{k\lambda}}\frac{\partial x_{k\lambda}}{\partial X_{l\tau}}(x_{ia} - \bar{x}_a) + \phi\,\frac{\partial x_{ia}}{\partial X_{l\tau}} \quad . \tag{3.11}$$

Using Cramer's rule, the set of equations for $\partial x_{k\lambda}/\partial X_{l\tau}$ are of the form

$$\frac{\partial x_{k\lambda}}{\partial X_{l\tau}} = \frac{E_{k\lambda,\,l\tau}}{D} \tag{3.12}$$

where D is the $3N$th-order determinant

$$\left|\frac{\partial\phi}{\partial x_{k\lambda}}(x_{ia} - \bar{x}_a) + \phi\,\delta_{ik}\,\delta_{a\tau}\right| \tag{3.13}$$

and $E_{k\lambda,\,l\tau}$ is D with the $k\lambda$ column replaced by the coefficients on the left-hand-side of eq. (3.11). For labeling the columns $k\lambda$ and the rows $i\alpha$, we fix first λ or α, which have the value 1, 2, 3 and then k or i are runned from 1 to N.

The determinant D is easily calculated (see ref. 2 where its elements are now given by the eq. (3.13)); we find

$$D = \phi^{3N-1}\Big(\phi + \sum_{j=1}^{N}\sum_{\beta=1}^{3}\frac{\partial\phi}{\partial x_{j\beta}}\,\bar{x}_{j\beta}\Big) \tag{3.14}$$

where $\bar{x}_{j\beta} = x_j - \bar{x}_\beta$. Using the fact that ϕ is a symmetric function of the difference of the coordinates, then we have

$$\sum_{j=1}^{N}\frac{\partial\phi}{\partial x_{j\beta}} = 0\,, \tag{3.15}$$

so the eq. (3.14) may also be written as

$$D = \phi^{3N-1}\left(\phi + \sum_{j=1}^{N} \sum_{\beta=1}^{3} \frac{\partial \phi}{\partial x_{j\beta}} x_{j\beta}\right). \tag{3.16}$$

On the other hand, for $E_{k\lambda,\, l\tau}$, using eq. (3.15), we obtain

$$E_{k\lambda,\, l\tau} = \phi^{3N-2}\left[\phi + \sum_{j=1}^{N} \sum_{\beta=1}^{3} x_{j\beta} \frac{\partial \phi}{\partial x_{j\beta}} (\delta_{kl} - \overline{\phi})\, \delta_{\lambda\tau} - \right.$$

$$\left. - x_{k\lambda} \frac{\partial \phi}{\partial x_{l\tau}}\right], \tag{3.17}$$

where $\overline{\phi} = (1 - \phi)/N$. Putting eqs. (3.14) and (3.17) in eq. (3.12), we have

$$\frac{\partial x_{k\lambda}}{\partial X_{l\tau}} = \frac{1}{\phi}\left[(\delta_{kl} - \phi)\, \delta_{\lambda\tau} - \frac{\overline{x}_{k\lambda}\, \partial\phi / \partial x_{l\tau}}{\phi + \sum_{j=1}^{N} \sum_{\beta=1}^{3} x_{j\beta} \frac{\partial \phi}{\partial x_{j\beta}}}\right]$$

Therefore,

$$\mathcal{L}_{i\alpha j\beta} = \sum_{l=1}^{N} \sum_{\tau=1}^{3} \frac{\partial x_{i\alpha}}{\partial X_{l\tau}} \frac{\partial x_{j\beta}}{\partial X_{l\tau}} = \frac{1}{\phi^2}\left[\delta_{\alpha\beta}\left(\delta_{ij} + \frac{\phi^2 - 1}{N}\right) - \right.$$

$$\left. - \frac{\overline{x}_{i\alpha}\phi'_{j\beta} + \overline{x}_{j\beta}\phi'_{i\alpha}}{\phi + \sum_{l=1}^{N} \sum_{\tau=1}^{3} x_{l\tau}\phi'_{l\tau}} + \overline{x}_{i\alpha}\overline{x}_{j\beta} \sum_{k=1}^{N} \sum_{\lambda=1}^{3} \frac{(\phi'_{k\lambda})^2}{\left(\phi + \sum_{l=1}^{N} \sum_{\tau=1}^{3} x_{l\tau}\phi'_{l\tau}\right)^2}\right], \tag{3.19}$$

and

$$B = \frac{\partial x_{k\lambda}}{\partial X_{l\tau}} = \left[\phi^{3N-4}\left(\phi + \sum_{j=1}^{N} \sum_{\beta=1}^{3} x_{j\beta}\phi'_{j\beta}\right)\right]^{-1}, \tag{3.20}$$

where $\phi'_{j\beta} = \partial\phi/\partial x_{j\beta}$.

Another immediate result coming from the symmetry condition on the function ϕ, which is a function of the difference of coordinates, is

$$\phi'_{j\beta} = \sum_{i=1}^{N} \frac{\partial\phi}{\partial r_{ij}} (x_{i\beta} - x_{j\beta})/r_{ij} \tag{3.21}$$

so that,

$$\sum_{j,\beta} x_{j\beta}\phi'_{j\beta} = \tfrac{1}{2} \sum_{i,\beta} \phi'_{r_{ij}} r_{ij} \tag{3.22}$$

and

$$\Sigma_\beta \phi'_{j\beta} G'_{j\beta} = \Sigma_{k,l} \frac{r_{ki} \cdot r_{lj}}{r_{kj} r_{lj}} \phi'_{r_{kj}} G'_{r_{lj}} \quad , \tag{3.23}$$

where $\phi'_{r_{ij}} = \partial\phi/\partial r_{ij}$ and G is an arbitrary function of the difference of coordinates.

In order to evaluate $W(r)$ we first note that eq. (3.7) can also be written as

$$W(r) = \sum_{i,j=1}^{N} \sum_{\alpha,\beta=1}^{3} B^{\frac{1}{2}} \frac{\partial}{\partial x_{i\alpha}} \left[\mathfrak{L}_{i\alpha j\beta} \frac{\partial}{\partial x_{j\beta}} (1/B)^{\frac{1}{2}} \right] \tag{3.24}$$

where we have used the relation (3.3). When using the eqs. (3.19), (3.22), we have

$$W(r) = B^{\frac{1}{2}} \left\{ \sum_{i,j}^{N} \sum_{\alpha=1}^{3} \frac{\partial}{\partial x_{ij\alpha}} \left(\frac{x_{ij\alpha}}{\phi^2_{r_{ij}} (\phi + \frac{1}{2} \Sigma_{k,l} r_{kl} \phi'_{r_{kl}})} \times \right.\right.$$

$$\left.\left. \times \left[\left(\frac{1}{B^{\frac{1}{2}}}\right)'_{r_{ij}} (\phi + \tfrac{1}{2} \sum_{k,l} r_{kl} \phi'_{r_{kl}}) - \tfrac{1}{2} \phi'_{r_{ij}} \sum_{k,l} r_{kl} \left(\frac{1}{B^{\frac{1}{2}}}\right)'_{r_{kl}} \right] \right) -$$

$$- \sum_{i=1}^{N} \sum_{\alpha=1}^{3} \frac{\partial}{\partial x_{i\alpha}} \left[\frac{\bar{x}_{i\alpha}}{\phi^2 (\phi + \frac{1}{2} \sum_{k,l} r_{kl} \phi'_{r_{kl}})^2} \right] \times$$

$$\times \left[\sum_{j,l,n} \phi'_{r_{lj}} \frac{r_{lj} \cdot r_{nj}}{r_{lj} r_{nj}} \left(\frac{1}{B^{\frac{1}{2}}} \right)'_{r_{nj}} (\phi + \sum_{k,s} r_{ks} \phi'_{r_{ks}}) \right.$$

$$\left. \left. - \tfrac{1}{2} \phi'_{r_{kj}} \left[\sum_{k,s} r_{ks} \left(\frac{1}{B^{\frac{1}{2}}} \right)'_{r_{ks}} \right] \right] \right\} . \tag{3.25}$$

where we have used the relations

$$\frac{\partial}{\partial x_{i\alpha}} - \frac{\partial}{\partial x_{j\alpha}} = 2 \frac{\partial}{x_{ij\alpha}} \tag{3.26}$$

$$x_{ij\alpha} = x_{i\alpha} - x_{j\alpha} \quad .$$

With respect to the potential $V(\boldsymbol{R}, \boldsymbol{P})$, if this is originally a short-range, strongly repulsive, or hard-core potential

$$V(\boldsymbol{R}, \boldsymbol{P}) = V(\boldsymbol{R}) = \begin{cases} \infty \ , & R \leqslant c \\ 0 & R > c \end{cases} \tag{3.27}$$

the transformation will eliminate the regions of the $3N$-dimensional configuration space in which any interparticle separation r_{ij} is less than the hard-core diameter c, as discussed in sec. 2. Therefore, due to eq. (3.27), the transformed potential will be $V_{ij}(r) = 0$ in the all the configuration space, in such a way that the transformed Hamiltonian, eq. (3.6), becomes in this case of a hard-core Hamiltonian,

$$H(\boldsymbol{r}, \boldsymbol{p}) = \sum_{i,j=1}^{N} \sum_{\alpha,\beta=1}^{3} p_{i\alpha} \mathfrak{L}_{i\alpha j\beta} p_{j\beta} + W(\boldsymbol{r}) \tag{3.28}$$

where $\mathfrak{L}_{i\alpha j\beta}$ is given by (3.19) and $W(r)$ by (3.25) and (3.20). The large effect of the original strong repulsive interaction is thus thrown into the new "metric" potential $W(r)$ and into the new coordinate and momentum potential $p\mathfrak{L}p$.

It is worth commenting at this stage that we have not specified the exact form of the function $g(r_{ij})$ except for the conditions given in (2.11). We have, therefore, a family of Hamiltonians, corresponding to the arbitrariness in the choice of the function $g(r)$, equivalent to the original hard-core Hamiltonian. Furthermore, eq. (3.28) represents a set of hermitian Hamiltonians amenable to the ordinary perturbation and variational techniques.

This method is accurate for calculation in which one can assume the existence of only few-body interaction terms. Of course, for a one-body isolated term, from eqs. (3.19) and (3.25), we obtain the unperturbed form:

$$H_i = \sum_{\alpha=1}^{3} p_{i\alpha}^2 \tag{3.29}$$

The pairwise limit is obtained if we consider obviously the two-body interaction terms, and then we put eq. (2.3), according to the eqs. (2.7) and (2.10) into the form

$$X_{ij\alpha} = x_{ij\alpha}\left(1 + \frac{c}{r_{ij} + \epsilon}\right) g(r_{ij}) \tag{3.30}$$

by changing to the relative coordinates $X_{ij\alpha}$ and $x_{ij\alpha}$ given by (3.26) and assuming that only the two-particles i, j are within a distance $r_{ij} < b$ so $g(r_{ik}), g(r_{jk}) \to 0$ for $k \neq i, j$. The transformation given by eq. (3.31) is the form assumed in previous investigations[3-6], where the systems are considered to be sufficiently dilute, so that the probability of a configuration with more than two particles within a distance b from another is negligible.

4. GENERAL REMARKS

Perhaps the most central quantity in the present theory is the function $g(r_{ij})$, related to the original trasnformation ϕ according to the discussion in sec. 2. This function seems to play the role of a radial distribution function like the one used in the theory of the liquid state[11]; and actually a theory more in accordance with first principles should include this de-

pendence of the probability distribution of the particles for the equilibrium situations. It should be emphasized that the derivation of the general form of the transformation function $\phi(\ldots x_{ia} \ldots)$ in sec. 2 is, up to a certain point, arbitrary, in such a way that, depending upon the form we choose for this function, strong statements about the behavior of the dynamical variables, the coordinates and momenta, and hence, about the class of transformed Hamiltonians, will be made.

Our approach in this problem has the advantage that analytic progress can be made although a lot of numerical work is still required. This method then becomes for those cases where the contribution of high order interacting terms is negligible; that is the price we have to pay when we put in balance accuracy and laborious mathematical computations. The value of this method is that a perturbation expansion can be considered to any order by keeping large enough interacting terms.

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RESUMEN

En este artículo se modifican las transformadas puntuales de muchas partículas, desarrolladas anteriormente for N.M. Witriol, para cubrir desde la transformación identidad – un cuerpo aislado – hasta la de N cuerpos interactuando, al variar las separaciones entre las partículas dentro de una distancia de corte escogida arbitrariamente. El método se usa para proporcionar Hamiltonianos de partículas que interaccionan fuertemente, que son equivalentes a los usuales.