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A mathematically rigorous formulation of the pseudopotential method

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Abstract

The Huang–Yang multipolar pseudopotential (see [K. Huang, Statistical Mechanics, Wiley, New York, 1963; K. Huang, C.N. Yang, Quantum-mechanical many-body problem with hard-sphere interaction, Phys. Rev. 105 (1957) 767–775]) is derived in a mathematically correct way using distribution theory. Up to recently, due to wrong numerical factors, only the first approximation term (the s-wave contribution) furnished correct results, and the conceptual validity of the higher approximations was in doubt, cf. [A. Derevianko, Revised Huang–Yang multipolar pseudopotential, Phys. Rev. A 72 (2005) 044701].

Keywords: Huang–Yang pseudopotential; Distribution theory; Perturbation of self-adjoint operators

1. Introduction

The pseudopotential method is an important technique to treat many-body problems, in particular Fermi and Bose gases at low temperatures. The aim of using the pseudopotential is to replace a complicated unknown potential, referring e.g. to the interaction of two particles, by a simple one that reproduces the same results, viz. energy values etc., in the long-range behaviour.

E. Fermi was among the first who replaced the exact interaction potential of a proton and a neutron by a substitution term, cf. [4, (80), p. 41]. Following Fermi's idea K. Huang and C.N. Yang tried to apply this technique to devise a pseudopotential which corresponds to the two-body system with hard-sphere interaction, i.e. $(\Delta_3 + k^2)\psi(x) = 0$ with $\psi|_{|x|=a} = 0$ was replaced by $(\Delta_3 + k^2)\psi(x) = U\psi(x)$, the pseudopotential U being an equivalent of the Dirichlet boundary condition. However, in their derivation, Huang and Yang omitted the numerical factor $\frac{1}{(2l+1)!}$ in [13, Eq. (9)] due to a slight calculational blunder. The difficult distributional differentiation formula in [13, Eq. (10)] is stated correctly (if interpreted in an appropriate distributional way), but without explanation. In his famous book [12], Huang repeated these calculations in detail. He corrected the missing factor $\frac{1}{(2l+1)!}$ (cf. [12, Eq. (B.8)]), but the purely heuris-

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tic and mathematically meaningless calculation of the distributional derivatives in Eq. (B.13) yields a false result. (This erroneous calculation is repeated in [17, (B.9), p. 205].) So both of the final formulas in [12] and [13] furnished incorrect results for $l \geqslant 1$.

This fact was observed later by several authors (cf. e.g. [18, p. 7]), and for a long time it was believed to be a fundamental flaw of the pseudopotential method. The reason for the false result in the book [12] was identified only recently by A. Derevianko (cf. [2]). He traces the mistake back to an erroneous application of the Gauss theorem. However, though his treatment yields the correct numerical factor, it likewise lacks mathematical rigour. We further point out that all these formulas contain terms which do not make sense without suitable distribution-theoretic interpretation (see Section 3 below). The Huang–Yang pseudopotential in the corrected form given by Derevianko (cf. [2, (1)]) is

$$U\psi(x) = -\frac{\hbar}{2\mu}\sum_{l,m}\frac{(2l+1)!!}{(2l)!!}\frac{\tan\eta_l}{k^{2l+1}}\cdot\frac{\delta(r)}{r^{l+2}}Y_{lm}(\Omega)\cdot\left(\frac{\partial}{\partial r}\right)^{2l+1}\left(r^{l+1}\psi_{lm}\right),$$
$$\psi(x) = \sum_{l,m}\psi_{lm}(r)Y_{lm}(\Omega), \qquad r = |x|,\ x = r\Omega. \tag{1}$$

The objective of this paper is to present the Huang–Yang pseudopotential in a mathematically correct way, since terms as $\frac{\delta(r)}{r^{l+2}}$ in (1) or $\frac{\delta^{(l)}(r)}{r^2}$—used in more recent representations, cf. [14]—cannot be interpreted in an unambiguous way without distribution theory. The distributional representation of the pseudopotential in (11) also shows that it is a Hermitian operator, in contrast to what has often been maintained (cf. [13, p. 769]; [17, B.1.2, p. 207]; [1, p. 2]).

The paper is organized in the following way. In Section 2, we derive a mathematically correct representation of the pseudopotential operator U for two-body hard-sphere interaction, cf. (8). Thereafter, in Section 3, we present a distributional interpretation of the (corrected) Huang–Yang pseudopotential (9), and show that the two representations are equivalent (Lemma 3). In Section 4, we then apply the pseudopotential operator to the eigenvalue problem which was studied as "illustrative example" in [13]. Instead of restricting the analysis to the case of spherically symmetric solutions (i.e. $l = 0$) as in the original paper, we calculate (with the help of the operator U) the first energy correction of the solution for general l, and we thereby check again the correctness of all terms of the pseudopotential.

Let us establish some notations. We always abbreviate the Euclidean norm $|x|$ of $x \in \mathbb{R}^3$ by r and write $x = r\Omega$ with Ω running over the unit sphere $\mathbb{S}^2$ in $\mathbb{R}^3$. The Heaviside function is denoted by H, i.e. $H(t) = 1$ for $t > 0$ and 0 else. The symbol O of Landau has its usual meaning: $f(t) = O(g(t))$ for $t \to 0$ means that f/g is bounded in a neighbourhood of 0. What considers the theory of distributions, we refer to [6,9,19]. In particular, $\langle\phi, T\rangle$ stands for the value of the distribution $T \in \mathcal{D}'$ on the test function $\phi \in \mathcal{D}$.

2. Distribution-theoretic derivation of the pseudopotential

2.1. Expansion in spherical harmonics

The Schrödinger equation for a system of two identical particles with hard-sphere interaction reduces in the center-of-mass system to the Helmholtz equation with a Dirichlet boundary condition:

$$\left(\Delta_3 + k^2\right)\psi(x) = 0 \quad \text{for } r > a,$$
$$\psi|_{r=a} = 0, \tag{2}$$

where $x \in \mathbb{R}^3$, $k \geqslant 0$, $r = |x|$, a is the hard-sphere diameter, and Δ_3 denotes the Laplace operator in three dimensions.

In order to solve this equation, we transcribe (2) into spherical coordinates and use the product-"ansatz"

$$\psi(x) = f(r)g(\vartheta, \varphi).$$

This yields

$$\left(f'' + \frac{2}{r}f' + k^2 f\right)g - \frac{1}{r^2}fBg = 0,$$

where B denotes the Laplace–Beltrami operator (cf. [20, §31, p. 419])

$$B : \mathcal{D}'\left(\mathbb{S}^2\right) \to \mathcal{D}'\left(\mathbb{S}^2\right) : T \mapsto -\Delta_3\left(T\left(\frac{x}{|x|}\right)\right)\Big|_{r=1}.$$

In spherical coordinates $\Omega = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta) \in \mathbb{S}^2$, we have

$$B = -\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\sin\vartheta\frac{\partial}{\partial\vartheta} - \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}.$$

The spherical harmonics $Y_{lm}(\Omega)$ are eigenfunctions of B with eigenvalues $l(l+1)$. $Y_{lm}(\Omega)$, $l \in \mathbb{N}_0$, $m = -l, \dots, l$, form an orthonormal basis in $L^2(\mathbb{S}^2)$, and more precisely we have (cf. [5, (A.31), (A.21)])

$$Y_{lm}(\Omega) = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\,P_l^m(\cos\vartheta)\,\mathrm{e}^{\mathrm{i}m\varphi},$$

$$P_l^m(t) = \frac{(-1)^m}{2^l l!}\big(1-t^2\big)^{\frac{m}{2}}\frac{\mathrm{d}^{l+m}}{\mathrm{d}t^{l+m}}\big(t^2-1\big)^l, \quad m = -l, \dots, l.$$

For $x = r\Omega \in \mathbb{R}^3$, $r = |x|$, $\Omega = \frac{x}{r} \in \mathbb{S}^2$, we define $Y_{lm}(x) := r^l Y_{lm}(\Omega)$. Then $Y_{lm}(x)$, $m = -l, \dots, l$, yield a basis of the harmonic polynomials of degree l.

The general solution of

$$f'' + \frac{2}{r}f' + \left(k^2 - \frac{l(l+1)}{r^2}\right)f = 0$$

is (cf. [7, 8.491.6])

$$\begin{aligned} f(r) &= C_1\frac{J_{l+\frac{1}{2}}(kr)}{\sqrt{kr}} + C_2\frac{J_{-l-\frac{1}{2}}(kr)}{\sqrt{kr}} \\ &= Aj_l(kr) + Bn_l(kr). \end{aligned} \tag{3}$$

Here $J_\nu(z)$ denote the Bessel functions of the first kind, meanwhile $j_l(kr)$ and $n_l(kr)$ are the so-called spherical Bessel and Neumann functions:

$$\begin{aligned} j_l(t) &:= \sqrt{\frac{\pi}{2t}}\,J_{l+\frac{1}{2}}(t) = \frac{t^l}{(2l+1)!!} + O\big(t^{l+2}\big), \quad t \to 0, \\ n_l(t) &:= (-1)^{l+1}\sqrt{\frac{\pi}{2t}}\,J_{-l-\frac{1}{2}}(t) = -\frac{(2l-1)!!}{t^{l+1}} + O\big(t^{-l+1}\big), \quad t \to 0 \end{aligned} \tag{4}$$

where $(2l+1)!! = 1 \cdot 3 \cdot 5 \cdots (2l+1)$.

We shall consider solutions $\psi(x)$ only whose expansions in spherical coordinates contain but a finite number of Y_{lm}, say such with $l \leqslant L$. With this restriction, the general solution of (2) is

$$\psi(x) = \sum_{l=0}^{L}\sum_{m=-l}^{l}\big(A_{lm}j_l(kr) + B_{lm}n_l(kr)\big)Y_{lm}(\Omega).$$

The boundary condition $\psi|_{r=a} = 0$ eliminates one of the constants:

$$A_{lm}j_l(ka) + B_{lm}n_l(ka) = 0 \quad \Rightarrow \quad B_{lm} = -A_{lm}\frac{j_l(ka)}{n_l(ka)},$$

and with $\tan\eta_l := \frac{j_l(ka)}{n_l(ka)}$, we obtain similarly to [13, (4), p. 768] the following:

$$\psi(x) = \sum_{l=0}^{L}\sum_{m=-l}^{l}A_{lm}\big(j_l(kr) - \tan\eta_l\, n_l(kr)\big)Y_{lm}(\Omega). \tag{5}$$

The next step consists in extending this solution to the region $r < a$. Since $j_l(kr)$ and $n_l(kr)$ are real analytic for $r \neq 0$, we can analytically continue the solution into the whole sphere $r < a$ excluding the point $x = 0$. (Let us observe in parentheses that this would not hold if we admitted infinitely many terms in (5). In fact, e.g. for $a = 1$ and $k = 0$ and fixed x_0 with $0 < |x_0| < 1$, the function $f(x) = \frac{1}{|x-x_0|} - \frac{|x_0|}{||x_0|^2x-x_0|}$ is harmonic in the region $1 < r < |x_0|^{-1}$ and vanishes on the unit sphere. Hence f can be expanded in this region into a series of the form $\sum_{l=0}^{\infty}\sum_{|m|\leqslant l}A_{lm}(r^l - r^{-l-1})Y_{lm}(\Omega)$. However, the analytic continuation of f across the unit sphere becomes infinite at x_0.)

In order to include the origin too, we have to discuss the terms $n_l(kr)Y_{lm}(\Omega)$ only, since

$$f(x) = j_l(kr)Y_{lm}(\Omega) = \frac{r^l k^l}{(2l+1)!!} Y_{lm}(\Omega) + O\big(r^{l+2}\big) Y_{lm}(\Omega)$$

is $\mathcal{C}^2$ and thus fulfills $(\Delta_3 + k^2) f = 0$ in all of $\mathbb{R}^3$. (Due to the ellipticity of the Helmholtz operator, f is real analytic also at the origin, cf. [10, Theorem 11.1.10, p. 67].)

In order to calculate $(\Delta_3 + k^2)\psi(x)$ in $\mathbb{R}^3$, we first interpret $n_l(kr)Y_{lm}(\Omega)$ as a distribution in $\mathcal{D}'(\mathbb{R}^3)$, which we denote by $\mathrm{vp}(n_l(kr)Y_{lm}(\Omega))$.

2.2. *Definition of* $\mathrm{vp}(n_l(kr)Y_{lm}(\Omega))$

The *principal value* $\mathrm{vp}\,\frac{1}{x} \in \mathcal{D}'(\mathbb{R}^1)$ is defined on a test function $\phi \in \mathcal{D}(\mathbb{R}^1) = \mathcal{C}_0^\infty(\mathbb{R}^1)$ in the following way (cf. [19, (II,2;29), p. 42]):

$$\left\langle \phi, \mathrm{vp}\,\frac{1}{x} \right\rangle := \lim_{\varepsilon \searrow 0} \int\limits_{|x|>\varepsilon} \frac{\phi(x)}{x}\,\mathrm{d}x \overset{\mathrm{supp}(\phi)\subseteq[-N,N]}{=} \int\limits_{-N}^{N} \frac{\phi(x)-\phi(0)}{x}\,\mathrm{d}x.$$

This means that $\mathrm{vp}\,\frac{1}{x}$ is the limit in $\mathcal{D}'(\mathbb{R}^1)$ of the locally integrable functions $\frac{H(|x|-\varepsilon)}{x}$ for $\varepsilon \searrow 0$. Similarly, we can define $\mathrm{vp}(n_l(kr)Y_{lm}(\Omega)) \in \mathcal{D}'(\mathbb{R}^3)$:

$$T := \mathrm{vp}\big(n_l(kr)Y_{lm}(\Omega)\big) := \lim_{\varepsilon \searrow 0} H(r-\varepsilon) n_l(kr) Y_{lm}(\Omega),$$

the limit being understood in $\mathcal{D}'(\mathbb{R}^3)$. Hence, if $\phi \in \mathcal{D}(\mathbb{R}^3)$, then

$$\langle \phi, T\rangle = \lim_{\varepsilon \searrow 0} \int\limits_{r \geqslant \varepsilon} \phi(x) n_l(kr) Y_{lm}(\Omega)\,\mathrm{d}x,$$

where $x = r\Omega$, $\Omega \in \mathbb{S}^2$, $r = |x|$.

Let us show that this limit exists and thus yields a distribution (by the weak-star sequential completeness of $\mathcal{D}'$, cf. [3, p. 100]). In fact, since $\int_{\varepsilon \leqslant |x| \leqslant N} x^\alpha Y_{lm}(\Omega)\,\mathrm{d}x = 0$ for $\alpha \in \mathbb{N}_0^3$, $|\alpha| < l$, cf. [3, 35, p. 170], we obtain, if $\phi \in \mathcal{D}(\mathbb{R}^3)$ with $\phi(x) = 0$ for $|x| \geqslant N$,

$$\begin{aligned}\langle \phi, T\rangle &= \lim_{\varepsilon \searrow 0} \int\limits_{\varepsilon \leqslant r \leqslant N} \left(\phi(x) - \sum_{|\alpha|<l} \frac{\partial^\alpha \phi(0)}{\alpha!} x^\alpha\right) n_l(kr) Y_{lm}(\Omega)\,\mathrm{d}x \\ &= \int\limits_{|x| \leqslant N} \left(\phi(x) - \sum_{|\alpha|<l} \frac{\partial^\alpha \phi(0)}{\alpha!} x^\alpha\right) n_l(kr) Y_{lm}(\Omega)\,\mathrm{d}x,\end{aligned}$$

the last integrand being an integrable function.

2.3. *Calculation of* $(\Delta_3 + k^2)\,\mathrm{vp}(n_l(kr)Y_{lm}(\Omega))$

Similarly as above, we can define the principal value $\mathrm{vp}(r^\lambda Y_{lm}(\Omega))$ for $\lambda \in \mathbb{C}$, if $\mathrm{Re}\,\lambda > -l-3$.

Lemma 1. *Let* $l \in \mathbb{N}_0$, $m = -l, \ldots, l$, *and* $\lambda \in \mathbb{C}$.

(a) *For* $\mathrm{Re}\,\lambda > -l-1$, *we have*

$$\Delta_3\,\mathrm{vp}\big(r^\lambda Y_{lm}(\Omega)\big) = (\lambda - l)(\lambda + l + 1)\,\mathrm{vp}\big(r^{\lambda-2} Y_{lm}(\Omega)\big).$$

(b) *If* $\mathrm{Re}\,\lambda > -l-1$ *and* $\lambda \notin \{2-l, 4-l, \ldots, -2+l\}$, *then*

$$\Delta_3\,\mathrm{vp}\big(r^\lambda Y_{lm}(\Omega)\big) = \frac{\lambda + l + 1}{(\lambda+l-2)(\lambda+l-4)\cdots(\lambda-l+2)}\,\mathrm{vp}\big(Y_{lm}(\partial) r^{\lambda+l-2}\big).$$

(c) $$\Delta_3\,\mathrm{vp}\big(r^{-l-1}Y_{lm}(\Omega)\big)=\frac{(-1)^{l-1}4\pi}{(2l-1)!!}Y_{lm}(\partial)\delta.$$

(Here $Y_{lm}(\partial)$ denotes the partial differential operator given by the harmonic polynomial $Y_{lm}(x)=r^lY_{lm}(\Omega)$, compare 2.1.*)*

Proof. (a) If $\operatorname{Re}\lambda>2$, then $r^\lambda Y_{lm}(\Omega)$ is a $\mathcal{C}^2$ function and the formula holds in the classical sense. Since the distribution-valued function

$$T_\lambda:\{\lambda\in\mathbb{C};\ \operatorname{Re}\lambda>-l-3\}\to\mathcal{D}'(\mathbb{R}^3):\quad \lambda\mapsto\mathrm{vp}\big(r^\lambda Y_{lm}(\Omega)\big)$$

is analytic (with derivative $\frac{\mathrm{d}T_\lambda}{\mathrm{d}\lambda}=\mathrm{vp}(r^\lambda\log r\,Y_{lm}(\Omega))$, cf. [6, p. 150]), the same differentiation formula holds for $\operatorname{Re}\lambda>-l-1$ by analytic extension.

(b) If $\operatorname{Re}\lambda>l+2$, then the formula

$$r^{\lambda-2}Y_{lm}(\Omega)=\frac{1}{(\lambda+l-2)(\lambda+l-4)\cdots(\lambda-l)}Y_{lm}(\partial)r^{\lambda+l-2}\tag{6}$$

holds in the classical sense: This is a special case of Hobson's formula (cf. [8, 79, (7), p. 127]). Let us indicate how formula (6) can be deduced rapidly by using the commutative graded algebra associated with the Laplace operator (cf. [11, p. 432]). In fact, if e_1,e_2,e_3 generate the commutative algebra Q over $\mathbb{C}$ with the relations $e_1^2+e_2^2+e_3^2=0$, and if $\nabla=\sum_{j=1}^3 e_j\partial_j$, $x=\sum_{j=1}^3 e_jx_j$, then (cf. [11, (7), p. 433])

$$\nabla^l r^\rho=\rho(\rho-2)\cdots(\rho-2l+2)x^lr^{\rho-2l}\tag{7}$$

and this yields

$$\begin{aligned}Y_{lm}(\partial)r^\rho&=\rho(\rho-2)\cdots(\rho-2l+2)Y_{lm}(x)r^{\rho-2l}\\&=\rho(\rho-2)\cdots(\rho-2l+2)r^{\rho-l}Y_{lm}(\Omega).\end{aligned}$$

This furnishes the equality in (b) of the lemma for large $\operatorname{Re}\lambda$, and this equation persists for $\operatorname{Re}\lambda>-l-1$ by analytic extension.

(c) The last assertion is deduced from the equation in (b) by approximating $-l-1$ by real λ from above:

$$\begin{aligned}\Delta_3\,\mathrm{vp}\big(r^{-l-1}Y_{lm}(\Omega)\big)&=\lim_{\lambda\searrow-l-1}\Delta_3\,\mathrm{vp}\big(r^\lambda Y_{lm}(\Omega)\big)\\&=\lim_{\lambda\searrow-l-1}\frac{\lambda+l+1}{(\lambda+l-2)(\lambda+l-4)\cdots(\lambda-l+2)}\mathrm{vp}\big(Y_{lm}(\partial)r^{\lambda+l-2}\big).\end{aligned}$$

Since $\lim_{\varepsilon\searrow0}\varepsilon r^{\varepsilon-3}=4\pi\delta$ in $\mathcal{D}'(\mathbb{R}^3)$, we obtain

$$\Delta_3\,\mathrm{vp}\big(r^{-l-1}Y_{lm}(\Omega)\big)=\frac{(-1)^{l-1}4\pi}{(2l-1)!!}Y_{lm}(\partial)\delta.\qquad\square$$

With the help of Lemma 1, we can calculate now $(\Delta_3+k^2)\,\mathrm{vp}(n_l(kr)Y_{lm}(\Omega))$ in the distributional sense:

Lemma 2. *Let $l\in\mathbb{N}_0$, $m=-l,\ldots,l$, and $k>0$. Then we have*

$$\big(\Delta_3+k^2\big)\,\mathrm{vp}\big(n_l(kr)Y_{lm}(\Omega)\big)=\frac{(-1)^l4\pi}{k^{l+1}}Y_{lm}(\partial)\delta.$$

Proof. Since

$$n_l(kr)=\sum_{j=0}^\infty d_jr^{2j-l-1}\quad\text{with } d_j:=\frac{(-1)^{l+j+1}\sqrt{\pi}\,k^{2j-l-1}}{\Gamma(j-l+\frac12)j!2^{2j-l}}$$

converges uniformly in compact subsets of $(0,\infty)$, we conclude that

$$T := \operatorname{vp}\big(n_l(kr)Y_{lm}(\Omega)\big) = \lim_{M\to\infty}\sum_{j=0}^{M} d_j \operatorname{vp}\big(r^{2j-l-1}Y_{lm}(\Omega)\big) \quad \text{in } \mathcal{D}'\big(\mathbb{R}^3\big).$$

Furthermore, for $2M-l-1>-3$,

$$\begin{aligned}
&\big(\Delta_3+k^2\big)\sum_{j=0}^{M} d_j \operatorname{vp}\big(r^{2j-l-1}Y_{lm}(\Omega)\big)\\
&\quad= d_0\Delta_3 \operatorname{vp}\big(r^{-l-1}Y_{lm}(\Omega)\big) + \sum_{j=1}^{M}\big(d_j\Delta_3 \operatorname{vp}\big(r^{2j-l-1}Y_{lm}(\Omega)\big) + k^2 d_{j-1}\operatorname{vp}\big(r^{2j-l-3}Y_{lm}(\Omega)\big)\big)\\
&\qquad + k^2 d_M r^{2M-l-1}Y_{lm}(\Omega)\\
&\quad= d_0\Delta_3 \operatorname{vp}\big(r^{-l-1}Y_{lm}(\Omega)\big) + k^2 d_M r^{2M-l-1}Y_{lm}(\Omega),
\end{aligned}$$

since the sum vanishes due to the first assertion in Lemma 1:

$$d_j\Delta_3 \operatorname{vp}\big(r^{2j-l-1}Y_{lm}(\Omega)\big) = d_j(2j-2l-1)2j \operatorname{vp}\big(r^{2j-l-3}Y_{lm}(\Omega)\big)$$

and

$$d_j(2j-2l-1)2j + k^2 d_{j-1} = 0.$$

Thus, by the third part of Lemma 1,

$$\big(\Delta_3+k^2\big)T = d_0\Delta_3 \operatorname{vp}\big(r^{-l-1}Y_{lm}(\Omega)\big) + \lim_{M\to\infty} k^2 d_M r^{2M-l-1}Y_{lm}(\Omega) = \frac{(-1)^l 4\pi}{k^{l+1}} Y_{lm}(\partial)\delta,$$

since $d_M r^{2M-l-1} \xrightarrow{M\to\infty} 0$, uniformly for bounded r, and $d_0 = -\frac{(2l-1)!!}{k^{l+1}}$, cf. [7, 8.339.3]. □

Hence, combining the results above we obtain

$$\big(\Delta_3+k^2\big)\psi(x) = \sum_{l=0}^{L}\sum_{m=-l}^{l} A_{lm}\frac{(-1)^{l+1}4\pi}{k^{l+1}}\tan\eta_l\, Y_{lm}(\partial)\delta.$$

Finally, we express the coefficient A_{lm} as a function of ψ (cf. [13]). Due to (5), the coordinates of $\psi(r\Omega)$ with respect to the orthonormal basis $Y_{lm}(\Omega)$ of $L^2(\mathbb{S}^2)$ are

$$\psi_{lm}(r) := \int_{\mathbb{S}^2}\psi(r\Omega)\overline{Y_{lm}(\Omega)}\,\mathrm{d}\Omega = A_{lm}\big(j_l(kr) - \tan\eta_l\, n_l(kr)\big),$$

cf. [13, (7), p. 768]. Recalling (4) we see that $r^{l+1}\psi_{lm}$ is $\mathcal{C}^\infty$ and it follows

$$A_{lm}\frac{k^l}{(2l+1)!!} = \frac{1}{(2l+1)!}\frac{\mathrm{d}^{2l+1}}{\mathrm{d}r^{2l+1}}\big(r^{l+1}\psi_{lm}\big)\Big|_{r=0}.$$

Let us remark that the factorial on the right-hand side is missing in the original article of Huang and Yang, cf. [13, (9), p. 768]. This error was corrected in Huang's book, cf. [12, Appendix B, (B.8)]. However, the final formula there is incorrect for other reasons, cf. the introduction.

Summarizing we obtain the following formula:

$$\big(\Delta_3+k^2\big)\psi(x) = 4\pi\sum_{l=0}^{L}\sum_{m=-l}^{l}\frac{(-1)^{l+1}}{(2l)!!\,k^{2l+1}}\tan\eta_l\cdot Y_{lm}(\partial)\delta\cdot\frac{\mathrm{d}^{2l+1}}{\mathrm{d}r^{2l+1}}\big(r^{l+1}\psi_{lm}\big)\Big|_{r=0}. \tag{8}$$

The right-hand side interpreted as an operator U applied to ψ is called *pseudopotential*.

3. Comparison with the Huang–Yang pseudopotential

The pseudopotential deduced by Huang and Yang (cf. [13, (12), p. 768]) is (if the missing factor $\frac{1}{(2l+1)!}$ is inserted)

$$\begin{aligned}(\Delta_3 + k^2)\psi(x) &= -\sum_{l=0}^{L}\sum_{m=-l}^{l} \frac{[(2l+1)!!]^2}{k^{2l+1}} \tan\eta_l \cdot \frac{\delta(r)}{r^{l+2}} Y_{lm}(\Omega) \cdot \frac{\mathrm{d}^{2l+1}}{\mathrm{d}r^{2l+1}}\big(r^{l+1}\psi_{lm}\big)\Big|_{r=0} \cdot \frac{1}{(2l+1)!} \\ &= -\sum_{l=0}^{L}\sum_{m=-l}^{l} \frac{(2l+1)!!}{(2l)!!\,k^{2l+1}} \tan\eta_l \cdot \frac{\delta(r)}{r^{l+2}} Y_{lm}(\Omega) \cdot \frac{\mathrm{d}^{2l+1}}{\mathrm{d}r^{2l+1}}\big(r^{l+1}\psi_{lm}\big)\Big|_{r=0} = U\psi. \end{aligned} \tag{9}$$

If we compare (9) with (8), we notice that it should hold

$$4\pi(-1)^{l+1} Y_{lm}(\partial)\delta \overset{!}{=} -(2l+1)!! \frac{\delta(r)}{r^{l+2}} Y_{lm}(\Omega).$$

In fact, it is possible to verify this equation by interpreting $\frac{\delta(r)}{r^{l+2}} Y_{lm}(\Omega)$ in an appropriate way:

Lemma 3. *For $l \in \mathbb{N}_0$, $m \in \mathbb{Z}$, $|m| \leqslant l$, define $S := \frac{\delta(r)}{r^{l+2}} Y_{lm}(\Omega) \in \mathcal{D}'(\mathbb{R}^3)$ by*

$$\frac{\delta(r)}{r^{l+2}} Y_{lm}(\Omega) := \lim_{\varepsilon \searrow 0} \frac{H(\varepsilon - r)}{\varepsilon} \operatorname{vp}\big(r^{-l-2} Y_{lm}(\Omega)\big).$$

(*Note that the multiplication of $H(\varepsilon - r)$ with $T = \operatorname{vp}(r^{-l-2} Y_{lm}(\Omega))$ is well-defined, since T is $\mathcal{C}^\infty$ outside the origin.*) *Then we have*:

(a) $\langle \phi, S\rangle = \lim_{r \searrow 0} r^{-l} \int_{\mathbb{S}^2} Y_{lm}(\Omega)\phi(r\Omega)\,\mathrm{d}\Omega$ *for* $\phi \in \mathcal{D}(\mathbb{R}^3)$;
(b) $S = \dfrac{4\pi(-1)^l}{(2l+1)!!} Y_{lm}(\partial)\delta.$

Proof. (a) For $\phi \in \mathcal{D}(\mathbb{R}^3)$ and $r \geqslant 0$, let us set

$$\chi(r) := \int_{\mathbb{S}^2} \phi(r\Omega) Y_{lm}(\Omega)\,\mathrm{d}\Omega.$$

From $\int_{\mathbb{S}^2} \Omega^\alpha Y_{lm}(\Omega)\,\mathrm{d}\Omega = 0$ for $|\alpha| < l$ and

$$\phi(x) = \sum_{|\alpha| \leqslant l} \frac{\partial^\alpha \phi(0)}{\alpha!} x^\alpha + O\big(|x|^{l+1}\big), \quad x \to 0,$$

we conclude that

$$\chi(r) = r^l \int_{\mathbb{S}^2} \sum_{|\alpha| = l} \frac{\partial^\alpha \phi(0)}{\alpha!} \Omega^\alpha Y_{lm}(\Omega)\,\mathrm{d}\Omega + O\big(r^{l+1}\big), \quad r \to 0.$$

On the other hand,

$$\big\langle \phi, H(\varepsilon - r)\operatorname{vp}\big(r^{-l-2} Y_{lm}(\Omega)\big)\big\rangle = \int_0^\varepsilon \chi(r) r^{-l}\,\mathrm{d}r$$

and hence

$$\langle \phi, S\rangle = \lim_{\varepsilon \searrow 0} \left\langle \phi, \frac{1}{\varepsilon} \int_0^\varepsilon \chi(r) r^{-l}\,\mathrm{d}r \right\rangle = \lim_{\varepsilon \searrow 0} r^{-l}\chi(r).$$

(b) As we have seen above,

$$\langle\phi, S\rangle = \lim_{r\searrow 0} r^{-l}\chi(r) = \int_{\mathbb{S}^2} \sum_{|\alpha|=l} \frac{\partial^\alpha\phi(0)}{\alpha!}\Omega^\alpha Y_{lm}(\Omega)\,\mathrm{d}\Omega$$
$$= \frac{1}{l!}\int_{\mathbb{S}^2} Y_{lm}(\Omega)\big((\Omega\cdot\nabla)^l\phi\big)(0)\,\mathrm{d}\Omega. \tag{10}$$

In the last equation, we used the multinomial formula. We shall deduce the explicit representation of S in (b) by calculating some spherical integrals in the same way as in [11, p. 445]. First of all we observe that, for two vectors $v, x \in \mathbb{R}^3$,

$$\int_{\mathbb{S}^2} (\Omega\cdot v)^l(\Omega\cdot x)^l\,\mathrm{d}\Omega = \frac{l!}{(2l)!}(v\cdot\nabla_x)^l \int_{\mathbb{S}^2}(\Omega\cdot x)^{2l}\,\mathrm{d}\Omega.$$

By rotational symmetry, we can set $x = (0, 0, |x|)$ in the integral on the right-hand side, and hence it yields

$$|x|^{2l}2\pi\int_0^\pi \cos^{2l}\vartheta\sin\vartheta\,\mathrm{d}\vartheta = \frac{4\pi|x|^{2l}}{2l+1}.$$

Therefore,

$$\int_{\mathbb{S}^2}(\Omega\cdot v)^l(\Omega\cdot x)^l\,\mathrm{d}\Omega = \frac{4\pi l!}{(2l+1)!}(v\cdot\nabla_x)^l|x|^{2l}.$$

If we use $e = (e_1, e_2, e_3)$ (e_i generate the commutative graded algebra associated with the Laplace operator, see [11, p. 432], and the proof of Lemma 1 above) instead of v and apply formula (7), we obtain

$$\int_{\mathbb{S}^2}(\Omega\cdot e)^l(\Omega\cdot x)^l\,\mathrm{d}\Omega = \frac{4\pi l!}{(2l+1)!}\left(\sum_{j=1}^3 e_j\partial_j\right)^l|x|^{2l} = \frac{4\pi l!(2l)!!}{(2l+1)!}\left(\sum_{j=1}^3 e_jx_j\right)^l.$$

Now we replace x by ∇ and conclude that

$$\int_{\mathbb{S}^2}(\Omega\cdot e)^l(\Omega\cdot\nabla)^l\,\mathrm{d}\Omega = \frac{4\pi l!(2l)!!}{(2l+1)!}\left(\sum_{j=1}^3 e_j\partial_j\right)^l.$$

Finally we use the representation

$$(\Omega\cdot e)^l = \left(\sum_{j=1}^3\Omega_je_j\right)^l = \sum_{\substack{\alpha\in\mathbb{N}_0^3\\ |\alpha|=l,\,\alpha_3=0,1}} Y_l^\alpha(\Omega)e^\alpha,$$

where $e^\alpha = e_1^{\alpha_1}e_2^{\alpha_2}e_3^{\alpha_3}$ and the coefficients $Y_l^\alpha(x)$, $|\alpha| = l$, $\alpha_3 = 0, 1$, form a maximal system of linearly independent homogeneous harmonic polynomials of degree l. Thus we obtain

$$\frac{1}{l!}\int_{\mathbb{S}^2} Y_{lm}(\Omega)(\Omega\cdot\nabla)^l\,\mathrm{d}\Omega = \frac{4\pi(2l)!!}{(2l+1)!}Y_{lm}(\partial).$$

Combining this result with (10) furnishes eventually

$$\langle\phi, S\rangle = \frac{4\pi(2l)!!}{(2l+1)!}\big(Y_{lm}(\partial)\phi\big)(0) = \left\langle\phi, \frac{4\pi(-1)^l}{(2l+1)!!}Y_{lm}(\partial)\delta\right\rangle. \qquad \square$$

Remark. The above calculations also yield a manifestly self-adjoint representation of the pseudopotential operator. In fact, from the proof of Lemma 3, we obtain

$$\frac{\mathrm{d}^{2l+1}}{\mathrm{d}r^{2l+1}}\big(r^{l+1}\psi_{lm}\big)\Big|_{r=0} = (2l+1)!\lim_{r\searrow 0} r^{-l}\psi_{lm}(r) = \frac{(2l+1)!}{l!}\int \overline{Y_{lm}(\Omega)}\big((\Omega\cdot\nabla)^l\psi\big)(0)\,\mathrm{d}\Omega = 4\pi(-1)^l(2l)!!\big\langle\psi, \overline{Y_{lm}(\partial)\delta}\big\rangle,$$

and hence, finally,

$$U\psi = -(4\pi)^2\sum_{l=0}^{L}\sum_{m=-l}^{l}\frac{\tan\eta_l}{k^{2l+1}}\cdot\big\langle\psi, \overline{Y_{lm}(\partial)\delta}\big\rangle\cdot Y_{lm}(\partial)\delta. \tag{11}$$

4. The "illustrative example" revisited

In order to become familiar with the pseudopotential derived above, we will apply it to the explicitly solvable *spherically symmetric* eigenvalue problem

$$\big(\Delta_3 + k^2\big)\psi = 0, \qquad a < r < R, \tag{12}$$

with the Dirichlet boundary condition

$$\psi|_{r=a} = \psi|_{r=R} = 0,$$

$0 < a < R$ being fixed, cf. [13, p. 769]. Since the region $V := \{x \in \mathbb{R}^3;\ a < r < R\}$ is bounded, the operator $-\Delta_3 : \mathcal{D}(V) \to L^2(V)$ is essentially self-adjoint and its Friedrichs extension $B : \mathring{W}_2^1(V) \to L^2(V)$ has pure point spectrum (cf. [20, Satz 29.1, p. 389]; [15, X.3, p. 176]). The eigenvalues $\epsilon = k^2$ of B, i.e. the energy, can be expanded in a power series with respect to a,

$$\epsilon = \epsilon^{(0)} + \epsilon^{(1)} + \cdots.$$

In (a) we shall calculate the first correction term $\epsilon^{(1)}$ from the explicit solution, and in (b) we shall check it by comparison with the eigenvalues of $-\Delta_3 + U$, where U denotes the pseudopotential on the right-hand side of (8) considered as an operator acting on functions on the ball $r < R$. These latter eigenvalues are calculated by means of perturbation theory [16]. For $l = 0$, i.e. for radially symmetric eigenstates respectively s-waves, this was done in [13, pp. 769, 770] and we will extend this analysis to general l.

(a) Thus we fix $l \in \mathbb{N}_0$ and $m \in \mathbb{Z}$ with $|m| \leqslant l$, and we consider only eigenvectors of B of the form

$$\psi(x) = A\left(j_l(kr) - \frac{j_l(ka)}{n_l(ka)}n_l(kr)\right)Y_{lm}(\Omega). \tag{13}$$

Due to the boundary condition $\psi|_{r=R} = 0$, the square root k of the eigenvalue must satisfy

$$\frac{j_l(kR)}{n_l(kR)} = \frac{j_l(ka)}{n_l(ka)}, \tag{14}$$

and the modulus of the constant A in (13) is determined by the normalization condition

$$\int\limits_{a<r<R}\big|\psi(x)\big|^2\,\mathrm{d}x = 1.$$

If $k_n(a)$ denotes the nth positive solution of (14), then $\kappa_n := k_n(0)$ fulfills $j_l(\kappa_n R) = 0$ and k_n has the expansion

$$k_n(a) = \kappa_n + Ca^m + O\big(|a|^{m+1}\big), \quad a \searrow 0.$$

At 0, the meromorphic function $f(t) := \frac{j_l(t)}{n_l(t)}$ has the Taylor expansion

$$f(t) = -\frac{t^{2l+1}}{(2l-1)!!(2l+1)!!} + O\big(t^{2l+3}\big), \quad t \to 0,$$

and hence

$$f\big(k_n(a)R\big) = f\big(k_n(a)a\big) = -\frac{\kappa_n^{2l+1}a^{2l+1}}{(2l-1)!!(2l+1)!!} + O\big(a^{2l+2}\big), \quad a \searrow 0,$$

implies

$$Ca^m Rf'(\kappa_n R) = -\frac{\kappa_n^{2l+1}a^{2l+1}}{(2l-1)!!(2l+1)!!},$$

i.e.

$$m = 2l+1 \quad \text{and} \quad C = -\frac{\kappa_n^{2l+1}}{(2l-1)!!(2l+1)!!Rf'(\kappa_n R)}.$$

From $j_l(\kappa_n R) = 0$ and [7, 8.472.2, 8.465.1, 8.477.1] we obtain

$$f'(\kappa_n R) = \frac{j_l'(\kappa_n R)}{n_l(\kappa_n R)}, \quad j_l'(\kappa_n R) = -j_{l+1}(\kappa_n R), \text{ and } n_l(\kappa_n R) = \frac{1}{\kappa_n^2 R^2 j_{l+1}(\kappa_n R)}$$

and hence

$$C = \frac{\kappa_n^{2l-1}}{(2l-1)!!(2l+1)!!R^3 j_{l+1}^2(\kappa_n R)}.$$

Thus $\epsilon = k_n(a)^2 = \kappa_n^2 + \epsilon_n^{(1)} + \cdots$, where κ_n is the nth positive root of $j_l(Rt)$ and the first energy correction term $\epsilon_n^{(1)}$ is given by

$$\epsilon_n^{(1)} = 2C\kappa_n a^{2l+1} = \frac{2\kappa_n^{2l}a^{2l+1}}{(2l-1)!!(2l+1)!!R^3 j_{l+1}^2(\kappa_n R)}. \tag{15}$$

(b) Let us next calculate the first energy correction using the pseudopotential. We extend the eigenfunction ψ in (13) to the ball $\{x \in \mathbb{R}^3;\ r = |x| < R\}$ as in Section 2, and we consider it then, in accordance with Eq. (9), as a solution of the equation $B\psi + U\psi = k^2\psi$, U denoting the operator on the right-hand side of (9). While this is not an eigenvalue problem (since k appears in a nonlinear way in U), we obtain one if we expand U with respect to a and retain just the first term. In fact,

$$\tan\eta_l = \frac{j_l(ka)}{n_l(ka)} = -\frac{k^{2l+1}}{(2l-1)!!(2l+1)!!}a^{2l+1} + O\big(a^{2l+2}\big), \quad a \searrow 0,$$

and hence

$$B\psi + U_1\psi = k^2\psi + O\big(a^{2l+2}\big) \quad \text{with } U_1\psi := \frac{a^{2l+1}}{(2l)!}\frac{\delta(r)}{r^{l+2}}Y_{lm}(\Omega)\cdot\frac{\mathrm{d}^{2l+1}}{\mathrm{d}r^{2l+1}}\big(r^{l+1}\psi_{lm}\big)\Big|_{r=0}.$$

The first energy correction term $\epsilon^{(1)}$ is given by the first term in the Rayleigh–Schrödinger series (cf. [16, Chapter XII]), i.e. $\epsilon^{(1)} = \langle U_1\psi_n^{(0)}, \overline{\psi_n^{(0)}}\rangle$, where $\psi_n^{(0)}$ is a normalized eigenvector of the unperturbed operator B with the (nondegenerate) eigenvalue κ_n^2. Evidently, $\psi_n^{(0)}$ reduces to $c_n j_l(\kappa_n r)Y_{lm}(\Omega)$. The absolute value of c_n is determined by (cf. [7, 6.521.1])

$$1 = \big\|\psi_n^{(0)}\big\|^2 = \int_{|x|<R} \big|\psi_n^{(0)}(x)\big|^2\,\mathrm{d}x = |c_n|^2\int_0^R j_l(\kappa_n r)^2 r^2\,\mathrm{d}r = \frac{|c_n|^2 R^3}{2} j_{l+1}^2(\kappa_n R),$$

i.e.

$$|c_n|^2 = \frac{2}{R^3 j_{l+1}^2(\kappa_n R)}.$$

From

$$\big(\psi_n^{(0)}\big)_{lm} = c_n j_l(\kappa_n r) = c_n\frac{\kappa_n^l r^l}{(2l+1)!!} + O\big(r^{l+2}\big), \quad r \to 0,$$

we obtain

$$\frac{\mathrm{d}^{2l+1}}{\mathrm{d}r^{2l+1}}\big(r^{l+1}\big(\psi_n^{(0)}\big)_{lm}\big)\Big|_{r=0} = c_n(2l)!!\kappa_n^l$$

and hence

$$U_1\psi_n^{(0)} = \frac{c_n\kappa_n^l a^{2l+1}}{(2l-1)!!}\cdot\frac{\delta(r)}{r^{l+2}}Y_{lm}(\Omega) = \frac{c_n\kappa_n^l a^{2l+1}}{(2l-1)!!}S,$$

where S is as in Lemma 3. Therefore, by (a) of Lemma 3, we finally infer

$$\begin{aligned}\epsilon_n^{(1)} = \big\langle U_1\psi_n^{(0)}, \overline{\psi_n^{(0)}}\big\rangle &= \frac{|c_n|^2\kappa_n^l a^{2l+1}}{(2l-1)!!}\big\langle j_l(\kappa_n r)\overline{Y_{lm}(\Omega)}, S\big\rangle \\ &= \frac{|c_n|^2\kappa_n^l a^{2l+1}}{(2l-1)!!}\lim_{r\searrow 0} r^{-l} j_l(\kappa_n r)\int_{\mathbb{S}^2} Y_{lm}(\Omega)\overline{Y_{lm}(\Omega)}\,\mathrm{d}\Omega \\ &= \frac{|c_n|^2\kappa_n^{2l} a^{2l+1}}{(2l-1)!!(2l+1)!!} = \frac{2\kappa_n^{2l} a^{2l+1}}{(2l-1)!!(2l+1)!!R^3 j_{l+1}^2(\kappa_n R)}\end{aligned}$$

in accordance with Eq. (15). Similarly, the first error term $\psi_n^{(1)}$ of the wave function ψ_n can be calculated from the formula

$$\psi_n^{(1)} = \sum_{i\neq n}\frac{\langle\overline{\psi_i^{(0)}}, U_1\psi_n^{(0)}\rangle}{\kappa_n^2-\kappa_i^2}\,\psi_i^{(0)}, \tag{16}$$

cf. [13, p. 770], for the case $l=0$. The sum in (16) represents just the Fourier–Bessel expansion (cf. [21, p. 381]) of $\psi_n^{(1)}$, which, by (13), has the form

$$\psi_n^{(1)} = a^{2l+1}\big[\alpha_n j_l(\kappa_n r) + \beta_n r j_l'(\kappa_n r) + \gamma_n n_l(\kappa_n r)\big]\cdot Y_{lm}(\Omega)$$

for suitable constants $\alpha_n, \beta_n, \gamma_n$.

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