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Research Article

Dirac quantization with constraints within intrinsic geometry

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Abstract

For motion constrained to a two-dimensional surface in three-dimensional Euclidean space, motion with respect to intrinsic geometry is quantized. The case of the helicoid is investigated here which is a minimal surface. It is shown how quantization can be carried out by including a geometrically induced potential and correction in the Hamiltonian.

Keywords: curvature; vector field; Hamiltonian; quantization; metric; constraints.

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1. Introduction

The study of quantum motion on a two-dimensional curved surface has been a subject of interest recently. The motion of a particle in a one or two-dimensional subset of Cartesian three-dimensional space is a problem which has come down by way of classical mechanics. It is often treated by means of the Newtonian approach as moving freely but subjected to spatial forces its velocity along a particular set of directions. There is also the Lagrangian approach in which the constraint is introduced from the beginning through generalized coordinates [1, 7, 10]. The standard parametrization $\mathbf{r}(q^1, q^2)$ of a two-dimensional surface is given by

$$\mathbf{r}(q^1, q^2) = (x(q^1, q^2), y(q^1, q^2), z(q^1, q^2)). \tag{1}$$

In (1), (q^1, q^2) is denoted q^μ where $\mu = 1, 2$ and $\mathbf{r}^\mu = g^{\mu\nu}\mathbf{r}_\nu = g^{\mu\nu}\,\partial_\nu \mathbf{r} = g^{\mu\nu}\partial\mathbf{r}/\partial q^\nu$. The metric tensor is given as $g_{\mu\nu} = \partial_\mu \mathbf{r} \cdot \partial_\nu \mathbf{r}$. At $\mathbf{r}$ the normal vector is $\mathbf{n} = (n_x, n_y, n_z)$ and $M\mathbf{n}$ denotes the mean curvature vector field. There exist two geometric invariants at $\mathbf{r}$. There is the mean curvature M and along with this, the gaussian curvature K. These respectively characterize the extrinsic and intrinsic curvature.

The objective here is to look at one problem quantum mechanically, and to do this, it should be possible to produce a Hamiltonian [5, 11, 12, 14]. A procedure has been proposed by de Witt [9] which requires the quantum kinetic energy operator be proportional to the Laplace-Beltrami operator Δ_{LB} for the surface

$$T_k = -\frac{\hbar^2}{2m}\,\Delta_{LB}. \tag{2}$$

A two-dimensional surface can be more realistically considered as a three-dimensional shell whose thickness is negligible in comparison with the dimensions of the entire system. There are two methods for calculating on this surface. First thinking of the surface as a limiting case of a curved shell or uniform thickness δ, where the limit $\delta \to 0$ is considered. The second method is referred to as the confining procedure for studying motion on a two-dimensional surface embedded in three dimensions.

It was da Costa [8] who considered the motion of a particle rigidly bound to a surface and showed that a part of the Hamiltonian should result from a geometrically induced potential. The confining procedure is applied to the momentum operator $\mathbf{P} = -i\hbar\nabla$ and it is found that the resultant momentum on the surface with normal vector $\mathbf{n}$ is

$$\mathbf{P} = -i\hbar\left(\mathbf{r}^\mu \partial_\mu + M\mathbf{n}\right) \tag{3}$$

was put forward in 2007 by an entirely independent development of quantization of momentum on a two dimensional surface embedded in three-dimensional flat space. This momentum corresponds to the so-called standard parametrization of the two-dimensional surface. There was also found to be a geometrically induced confining potential which is given by

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$$V_g = -\frac{\hbar^2}{2m}(M^2 - K), \tag{4}$$

where K is the Gaussian curvature. For the helicoid, the curvature K is given by

$$K = -\frac{a^2}{(u^2 + a^2)^2}.$$

Another approach is canonical quantization whose fundamental hypotheses are that the fundamental quantum conditions between generalized coordinates x_μ and momenta p_ν with $\mu = 1, 2$, or Cartesian x_i and p_i preserve the same algebraic structure as they do in classical mechanics.

To generalize the quantum conditions, the commutator is modified and introduced in the form

$$[A, B] = i\hbar\{A, B\}_D,$$

for any pair of quantities A and B, and $\{A, B\}_D$ is the Dirac bracket for a system which has second-class constraints. It reduces to the usual Poisson bracket when the system is free of constraints. Some of the constraints may be superfluous, and a good generalization would be to include some quantum conditions into the fundamental category, so an enlarged canonical quantization procedure results and will be looked at here. The interaction of geometry and topology frequently manifests itself in the form of unusual electronic and magnetic properties of materials. For example, for electrons confined to a helicoid ribbon, potential (4) leads to the appearance of localized states at the rim of the helicoid [13].

There has recently appeared an example which seems to yield some inconsistencies in Dirac's procedure when the manifold is coordinatized intrinsically. It will be shown that this can be treated by including an additional contribution to V_g. It might be thought of as quantum mechanical in origin, as a particle confined to a surface immersed in three-dimensional space should be subjected to uncertainty relations normal or off the surface penetrating the ambient space. It also may account for why Dirac thought his procedure best used in Cartesian coordinates, as these are not intrinsically confined to the surface. So in three-dimensional Euclidean space, the Dirac procedure seems to be satisfactory [15].

2. Second-class constraints for the helicoid-classical case

The helicoid can be coordinatized by means of two local coordinates $u \in (-\infty, \infty)$ and $v \in (-\infty, \infty)$ accompanied by a real parameter a which characterizes the pitch as

$$\mathbf{r}(u, v) = (u \cos\, v, u \sin\, v, a\, v). \tag{5}$$

First the classical mechanics is given for the motion on the helicoid within Dirac's theory of second class constraints. The quantum case is turned to next. In classical mechanics, the theory appears nothing surprising. However, after the transition to quantum mechanics, it seems to become self-contradictory. The main contribution here is to explain or account for this problem in physical terms.

The Lagrangian L in terms of local coordinates is given by

$$L = \frac{1}{2}m\big(\dot v^2(r^2 + u^2) + 2r\dot r\, v\dot v + \dot r^2 v^2 + \dot u^2\big) - \lambda\,(r - a). \tag{6}$$

A Lagrange multiplier λ is used in (6) to enforce constrained motion on the surface. Moreover, λ can be treated as an additional dynamical variable. The Lagrangian is singular because it does not contain the time derivative or velocity $\dot\lambda$. Dirac's theory of quantization with constraints is required. The canonical momenta which are conjugate to r, u, v and λ are calculated first,

$$\begin{gathered} p_r = \frac{\partial L}{\partial \dot r} = mv(r\dot v + v\dot r), \\ p_u = \frac{\partial L}{\partial \dot u} = m\dot u, \\ p_v = \frac{\partial L}{\partial \dot v} = m(r^2\dot v + rv\dot r + u^2\,\dot v) = m((r^2 + u^2)\dot v + r\dot r\, v), \\ p_\lambda = \frac{\partial H}{\partial \dot\lambda} = 0. \end{gathered} \tag{7}$$

The final equation in (7) generates the primary constraint

$$\varphi_1 = p_\lambda \equiv 0.$$

Solving this system of equations for the variables $\dot{r}$, $\dot{u}$ and $\dot{v}$, we obtain

$$\dot{r} = \frac{1}{mu^2v^2}(p_r u^2 - rvp_v + r^2 p_r), \qquad \dot{u} = \frac{p_u}{m}, \qquad \dot{v} = \frac{1}{mu^2 v}(vp_v - rp_r). \tag{8}$$

The primary Hamiltonian is then obtained from L and (8) as

$$H = H_p = \dot{r}p_r + \dot{v}p_v + \dot{u}p_u - L$$

$$= \frac{1}{2\,mu^2v^2}\left[(r^2+u^2)p_r^2 - 2rv\,p_r\,p_v + (p_v^2 + u^2 p_u^2)\,v^2\right] + \lambda(r-a) + \eta\,p_\lambda.$$

The variable η is also a Lagrange multiplier which guarantees that this Hamiltonian is defined on the symplectic manifold. The Poisson bracket $\{f,g\}$ is defined as follows

$$\{f,g\} = \frac{\partial f}{\partial q_k}\frac{\partial g}{\partial p_k} + \frac{\partial f}{\partial \lambda}\frac{\partial g}{\partial p_\lambda} - \left(\frac{\partial f}{\partial p_k}\frac{\partial g}{\partial q_k} + \frac{\partial f}{\partial p_\lambda}\frac{\partial g}{\partial \lambda}\right).$$

To compute Poisson brackets, let us suppose $q_1 = r$, $q_2 = u$, $q_3 = v$ and $p_1 = p_r$, $p_2 = p_u$ and $p_3 = p_v$.

The complete system of secondary constraints can now be determined to be

$$\varphi_2 = \{\varphi_1, H\} = \{p_\lambda, H\} = a - r \approx 0,$$

$$\varphi_3 = \{\varphi_2, H\} = \{a-r, H\} = \frac{\partial}{\partial r}(a-r)\frac{\partial H}{\partial p_r} = -\frac{1}{2mu^2v^2}\left((2(r^2+u^2)p_r - 2rvp_v\right) \approx 0,$$

$$\varphi_4 = \{\varphi_3, H\} = \frac{r^2+u^2}{mu^2v^2}\,\lambda + 2\frac{(p_v v - p_r r)(p_r(r^2+u^2) - ruv^2\,p_u - rv\,p_v)}{m^2u^4v^4} \approx 0.$$

The $\approx$ means to vanish as a constraint, or weak equality. It defines a subspace in phase space and can be set to zero after all brackets have been worked out. Solving the constraints $\varphi_3 \approx 0$ and $\varphi_4 \approx 0$ on the constraint surface for the variables p_r and λ, it follows that

$$p_r = \frac{rv}{r^2+u^2}\,p_v,$$

$$\lambda = 2\frac{(p_r r - p_v v)(p_r r^2 + p_r u^2 - p_v rv - p_u ru\,v^2)}{mu^2r^2(r^2+u^2)} = \frac{2ruv}{m(r^2+u^2)^2}\,p_u p_v.$$

These results show that on the surface of the helicoid $r = a$ the dynamical variable λ is determined. By the conservation condition of the secondary constraint φ_4, the Lagrange multiplier η can be determined.

The Dirac bracket is defined for the two variables A and B in terms of their Poisson bracket as follows

$$\{A,B\}_D = \{A,B\} - \{A,\varphi_\alpha\}\,C^{-1}_{\alpha\beta}\,\{\varphi_\beta, B\}, \tag{9}$$

The 4×4 matrix $C = (C_{\alpha\beta})$ has matrix elements which are defined in terms of the φ_α to be as $C_{\alpha\beta} = \{\varphi_\alpha, \varphi_\beta\}$ with $\alpha,\beta = 1,\dots,4$, or explicitly as

$$\mathbf{C} = \begin{bmatrix} 0 & C_{12} & C_{13} & C_{14} \\ C_{21} & 0 & C_{23} & C_{24} \\ C_{31} & C_{32} & 0 & C_{34} \\ C_{41} & C_{42} & C_{43} & 0 \end{bmatrix} \tag{10}$$

The matrix elements in (10) are given be

$$C_{12} = \{\varphi_1, \varphi_2\} = \{p_\lambda, a-r\} = 0, \quad C_{13} = \{p_\lambda, \varphi_3\} = 0,$$

$$C_{14} = \{p_\lambda, \varphi_4\} = -\frac{r^2+u^2}{mu^2v^2}, C_{23} = \frac{r^2+u^2}{mu^2v^2},$$

$$C_{24} = -2\frac{r^2v\,p_u + up_v}{m^2u^3v^3}, \quad C_{34} = 2\frac{2u^2r^2p_u + 2uvr^2p_v + 3r^4p_u - u^4p_u}{m^3u^3v^3\,(r^2+u^2)^2}\,p_v.$$

The inverse matrix C^{-1} is required to evaluate the Dirac bracket (9), and it is given by

$$C^{-1} = \begin{bmatrix} 0 & C^{-1}_{12} & C^{-1}_{13} & C^{-1}_{14} \\ -C^{-1}_{12} & 0 & C^{-1}_{23} & 0 \\ -C^{-1}_{13} & -C^{-1}_{23} & 0 & 0 \\ -C^{-1}_{14} & 0 & 0 & 0 \end{bmatrix}$$

The matrix elements for matrix C^{-1} will appear explicitly when the inverse of the matrix C is calculated. The following matrix elements are found

$$C_{12}^{-1} = \frac{2uvp_v(3a^4p_u + 2a^2u(up_u + vp_v) - u^4p_u)}{m(u^2+a^2)^4},$$

$$C_{23}^{-1} = \frac{2uv(a^2vp_u + up_v)}{(u^2+a^2)^2},$$

$$C_{14}^{-1} = -C_{23}^{-1} = \frac{mu^2v^2}{u^2+a^2}.$$

Therefore, the generalized positions $q^\mu = (u, v)$ and momenta $p_\nu = (p_u, p_v)$ satisfy the following Dirac brackets,

$$\{q^\mu, q^\nu\}_D = 0, \qquad \{p_\mu, p_\nu\}_D = 0, \qquad \{q^\mu, p_\nu\}_D = \delta^\mu_\nu.$$

Explicitly for example, these can be verified in the following way,

$$\{u, v\}_D = -\{u, \varphi_\alpha\}C_{\alpha\beta}^{-1}\{\varphi_\beta, v\} = -\frac{\partial \varphi_\alpha}{\partial p_u} C_{43}^{-1} \frac{\partial \varphi_3}{\partial p_v} = 0,$$

$$\{p_u, p_v\}_D = -\{p_u, \varphi_\alpha\}C_{\alpha\beta}^{-1}\{\varphi_\beta, p_v\} = -\{p_u, \varphi_3\}C_{34}^{-1}\{\varphi_4, p_4\} - \{p_u, \varphi_4\}C_{43}^{-1}\{\varphi_3, p_{\}} = 0,$$

$$\{u, p_u\}_D = -\{u, p_u\} - \{u, \varphi_\alpha\}C_{\alpha\beta}^{-1}\{\varphi_\beta, p_u\} = \{u, p_u\} - \{u, \varphi_4\}C_{43}^{-1}\{\varphi_3, p_u\} = 1.$$

Using the general form of the equation of motion for the variable f,

$$\dot{f} = \{f, H\}_D,$$

the equations of motion for the position variables u, v and their associated momenta p_u, p_v can be determined in the following way. The usual Hamiltonian H can be obtained from H_p by substituting the expression for p_r into H_p and applying the constraints. The usual form of the Hamiltonian is given by

$$H = \frac{1}{2m}\left(p_u^2 + \frac{p_v^2}{u^2+a^2}\right).$$

It can be seen that the Dirac theory for the classical motion on the helicoid is complete and consistent in itself.

Therefore, the brackets are found to yield the following equations of motion,

$$\dot{u} = \{u, H\}_D = \{u, H\} - \{u, \varphi_4\}C_{4\beta}^{-1}\{\varphi_\beta, H\} = \frac{p_u}{m},$$

$$\dot{v} = \{v, H\}_D = \{v, H\} - \{v, \varphi_\alpha\}C_{\alpha\beta}^{-1}\{\varphi_\beta, H\} = \frac{p_v}{m(u^2+a^2)},$$

$$\dot{p}_u = \{p_u, H\}_D = \{p_u, H\} - \{p_u, \varphi_\alpha\}C_{\alpha\beta}^{-1}\{\varphi_\beta, H\} = \frac{u}{m(u^2+a^2)^2}\,p_v^2,$$

$$\dot{p}_v = \{p_v, H\}_D = 0.$$

3. Quantum case

This system can now be studied from the quantum point of view. It is necessary to construct a quantum Hamiltonian. To this end one approach is to calculate the Laplace-Beltrami operator by calculating a metric for the surface and using it to calculate

$$\Delta_{LB}\phi = \frac{1}{\sqrt{g}}\frac{\partial}{\partial q^i}\left[\sqrt{g}g^{ij}\frac{\partial \phi}{\partial q^i}\right]. \tag{11}$$

In (11), (g_{ij}) are the components of the metric on the surface, (g^{ij}) its inverse and $g = \det(g_{ij})$. The physical T_k follows from (5) by using (2). Starting with the component representation of the helicoid, $\mathbf{r}(u, v) = (u\cos(v), u\sin(v), a\,v)$, the metric is

$$g_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & u^2+a^2 \end{bmatrix}$$

Clearly $\det(g) = u^2 + a^2$. The desired operator is found to be

$$\Delta_{LB}\phi = \frac{1}{\sqrt{u^2+a^2}}\left[\frac{\partial^2}{\partial u}\sqrt{u^2+a^2}\frac{\partial \phi}{\partial u} + \frac{\partial}{\partial v}\sqrt{u^2+a^2}\frac{1}{u^2+a^2}\frac{\partial \phi}{\partial v}\right]$$

$$= \frac{\partial^2 \phi}{\partial u^2} + \frac{u}{u^2+a^2}\frac{\partial \phi}{\partial u} + \frac{1}{u^2+a^2}\frac{\partial^2 \phi}{\partial v^2}.$$

It can also be determined by finding the geometric momenta on the surface from (3). Since the helicoid is a minimal surface $M = 0$ and we find

$$\begin{aligned} \hat{P}_1 &= -i\hbar \left(\cos v \frac{\partial}{\partial u} - \frac{u}{u^2+a^2} \sin v \frac{\partial}{\partial v} \right), \\ \hat{P}_2 &= -i\hbar \left(\sin v \frac{\partial}{\partial u} + \frac{u}{u^2+a^2} \cos v \frac{\partial}{\partial v} \right), \\ \hat{P}_3 &= -i\hbar \frac{a^2}{u^2+a^2} \frac{\partial}{\partial v}. \end{aligned} \tag{12}$$

The Hamiltonian is calculated based on the results of (12) and it is

$$T_k = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial u^2} + \frac{u}{u^2+a^2}\frac{\partial}{\partial u} + \frac{1}{u^2+a^2}\frac{\partial^2}{\partial v^2} \right).$$

Another way to get this is to begin with the more general metric

$$g = (r^2+a^2) dv \otimes dv + rv\, dr \otimes dv + rv\, dv \otimes dr + v^2 dr \otimes dr + du \otimes du.$$

It is required to determine three linearly independent Killing vector fields for this metric. This means the Lie derivative of the metric with respect to the vector field must vanish. To carry this out, let X be a vector field with unknown coefficients f, h, k which depend on the coordinates r, u, v

$$X = f\frac{\partial}{\partial r} + h\frac{\partial}{\partial u} + k\frac{\partial}{\partial v} = f\mathbf{e}_1 + h\mathbf{e}_2 + k\mathbf{e}_3.$$

This also serves to define the basis set $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\} = \{\partial/\partial r, \partial/\partial u, \partial/\partial v\}$. These three functions are determined by requiring that the Lie derivative of the metric vanish

$$\mathcal{L}_X\, g = 0.$$

After a calculation [4] a coupled system of six partial differential equations is obtained for these functions from (12). Solving the system and assigning the integration constants the following Noether momenta vector fields result

$$\begin{gathered} P_{n1} = -\frac{r}{uv}\cos v\mathbf{e}_1 + \sin v\, \mathbf{e}_2 + \frac{1}{u}\cos v\mathbf{e}_3, \quad P_{n2} = \frac{r}{uv}\sin v\mathbf{e}_1 + \cos v\,\mathbf{e}_2 - \frac{1}{u}\sin v\, \mathbf{e}_3, \\ P_{n3} = \frac{1}{v}\mathbf{e}_1. \end{gathered} \tag{13}$$

The same notation is used as above since the results will be identical. To transform this to the constrained system, in which $r = a$ is applied, note that the classical momenta p_r and p_v are related as

$$p_r = \frac{rv}{u^2+r^2}\, p_v, \qquad r = a.$$

Putting the constraints in (13), the P_{ni} in (13) take the form

$$P_1 = \sin v\mathbf{e}_2 + \frac{u}{u^2+a^2}\cos\, v\mathbf{e}_3 \quad P_2 = \cos v\mathbf{e}_2 - \frac{u}{u^2+a^2}\sin v\mathbf{e}_3, \quad P_3 = \frac{a}{a^2+u^2}\mathbf{e}_3.$$

Identifying these as operators, the quantum momenta result,

$$\begin{aligned} \hat{P}_1 &= -i\hbar \left(\sin v \frac{\partial}{\partial u} + \frac{u}{u^2+a^2} \cos v \frac{\partial}{\partial v} \right), \\ \hat{P}_2 &= -i\hbar \left(\cos v \frac{\partial}{\partial u} - \frac{u}{u^2+a^2} \sin v \frac{\partial}{\partial v} \right), \\ \hat{P}_3 &= -i\hbar \frac{a}{u^2+a^2} \frac{\partial}{\partial v}. \end{aligned} \tag{14}$$

The results in (10) are identical with the results given in (12). Combining momenta (14) leads to the same kinetic Hamiltonian

$$T_k = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial u^2} + \frac{u}{u^2+a^2}\frac{\partial}{\partial u} + \frac{1}{u^2+a^2}\frac{\partial^2}{\partial v^2} \right). \tag{15}$$

The total Hamiltonian is now formed by including the geometrically induced potential and any other correction terms along with (15) [2,3]. This potential is denoted $U(u,v)$ depending just on the coordinates u, v and the total Hamiltonian is given by

$$H=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial u^2}+\frac{u}{u^2+a^2}\frac{\partial}{\partial u}+\frac{1}{u^2+a^2}\frac{\partial^2}{\partial v^2}+U(u,v)\right). \tag{16}$$

To study the quantum equations of motion now, it is required that the Dirac bracket be replaced by a commutator bracket multiplied by $i/\hbar$ as here

$$\dot{Q}=\frac{i}{\hbar}[H,Q].$$

From the Dirac brackets the fundamental commutator are given as follows

$$[q^{\mu},q^{\nu}]=0, \qquad [p_{\mu},p_{\nu}]=0, \qquad [q^{\mu},p_{\nu}]=i\hbar\,\delta^{\mu}_{\nu}.$$

Using Hamiltonian (16), the quantum equations for u and v take the form

$$[u,H]=i\frac{\hbar}{m}p_u, \qquad [v,H]=i\frac{\hbar}{m}\frac{p_v}{u^2+a^2}.$$

Using H given by (16), it is found that [6]

$$[u,H]=\frac{\hbar^2}{m}\left(\frac{\partial}{\partial u}+\frac{u}{2(u^2+a^2)}\right)=i\frac{\hbar}{m}p_u, \qquad [v,H]=\frac{\hbar^2}{m}\left(\frac{1}{u^2+a^2}\frac{\partial}{\partial v}\right)=i\frac{\hbar}{m}\frac{p_v}{u^2+a^2}.$$

This gives a explicit form for the operators p_u and p_v

$$p_u=-i\hbar\left(\frac{\partial}{\partial u}+\frac{u}{2(u^2+a^2)}\right), \qquad p_v=-i\hbar\frac{\partial}{\partial v}. \tag{17}$$

Finally, we can calculate directly the two quantum commutator $[p_u,H]$ and $[p_v,H]$ with this Hamiltonian with the following results

$$[p_u,H]=i\hbar\{p_u,H\}_D, \qquad [p_v,H]=0,$$

provided the potential function $U(u,v)$ in H is taken to have the form

$$U(u,v)=\frac{2a^2-u^2}{4(u^2+a^2)^2}=K+\frac{6a^2-u^2}{4(u^2+a^2)^2}.$$

It is also the case that if momenta (17) to construct a Hamiltonian, the result from (16) is recovered.

4. Conclusions

The behavior of quantum systems constrained to move on a surface has been of interest to study for some time. Also, the topic of quantum mechanics in curved space has been looked at via different methods such as canonical quantization, path integral method and Dirac approach. An investigation of the quantum motion of a particle on the helicoid has been carried out here. On a curved surface no exact Cartesian coordinate system within intrinsic geometry is present. In effect, an enlarged canonical quantization procedure has been proposed in which positions, momenta and Hamiltonian are simultaneously quantized. It has been proposed that an inconsistency within Dirac theory occurs and it has been proposed that this can be accounted for by means of quantum correction to the surface. Future work might be to see if these results can be attained another way such as by using string theory, or whether this kind of calculation can be fitted in to drive a string theory calculation. It remains to see whether this modified potential can better account for experimental results.

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