General properties of ground-state energies of relativistic two-body Hamiltonians with Coulomb and Yukawa potentials

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Estimates and critical stability thresholds characterizing the ground-state energies have been established with the help of a quasiclassical generalization of the virial theorem proposed previously. This enables us to evaluate ground-state energies in terms of the minima of corresponding Hamiltonian dispersions. Relativistic ($m_1 = m_2 = m_0$) and nonrelativistic two-body Hamiltonians with Coulomb and Yukawa potentials have been considered. For relativistic spin-$\frac{1}{2}$ particles, as well as for the nonrelativistic ones, the calculations proceed by fixing to unity the underlying phase-space quantum.

I. INTRODUCTION

The nonrelativistic bound-state energies for Debye-Hückel (Yukawa) potentials have been analyzed by use of perturbative,[1] analytic perturbative,[2] variational,[3] scaling variational,[4] numerical intergration,[5] nonlinear numerical,[6] and other methods. Summation methods of perturbation series,[7] and ϵ expansions,[8] as well as asymptotic methods combined with normalizability,[9] should also be included. Superpositions of Coulomb and power potentials,[10] or Coulomb and Yukawa potentials,[11] have also been considered. In this paper we shall continue such studies by analyzing the ground-state energies (GSE's) for Coulomb and Yukawa potentials, this time in terms of a suitable quasiclassical generalization of the quantum-mechanical (QM) virial theorem proposed previously.[12] This enables us to define quite simply the GSE as

$$\mathscr{E} = \min \delta H(r) , \quad (1)$$

provided that the above minimum exists and takes finite values. Equation (1) generalizes some usual uncertainty-relation estimates assumed provisionally on this subject.[13] Here $\delta H(r) = H(r, \hbar d_0/r)$ is the so-called QM dispersion[14] of the spherically symmetrical Hamiltonian $H(r,p)$. Next $d_0 \sim 1$ ($d_0 > 0$) denotes the underlying phase-space quantum, whereas $r = |\mathbf{x}|$ and $p = |\mathbf{p}|$.

One proceeds with use of basic non-Hermitian constituents of usual observables as well as suitable probe functions.[15] Such constituents come from the quasiclassical $\hbar \rightarrow 0$ limit of expansions of the usual physical phase-space observables $\hat{f}(r,p)$, with respect to basic r, and $\hat{a} = i\hbar \mathbf{x} \cdot \partial/\partial \mathbf{x}$ operators, in which the $\hat{a}$ dilation operators are placed on the right of each term for purposes of nonsymmetrical ordering.[16] So far, nonintegrable powerlike probe functions have been invoked. In spite of its simplicity, the present method enables us to establish reasonable estimates and typical stability constraints as well as general properties characterizing the GSE's for single- or two-particle systems.[15] For the sake of generality we shall consider the relativistic (R) two-particle ($m_1 = m_2 = m_0$) Hamiltonian

$$H_1(r,p) = 2p_0 + V(r) , \quad (2)$$

in which the vector potential is the above-mentioned superposition

$$V(r) = -(\alpha\hbar/r) - (g\hbar/r)\exp(-\mu r/\hbar) \quad (3)$$

of Coulomb and Yukawa potentials. Next we shall perform detailed calculations for $\alpha = 0$ and $g = 0$, respectively. The corresponding nonrelativistic (NR) Hamiltonian is

$$H_2(r,p) = (p^2/m_0) + V(r) , \quad (4)$$

as usual. In the equations, $\alpha > 0$, $g > 0$, $\mu > 0$ is a mass scale and $p_0 = (p^2 + m_0^2)^{1/2}$. In the R case we can revert to the single-particle problem by performing the rescalings $\alpha \rightarrow 2\alpha$ and $g \rightarrow 2g$ and dividing the results by 2. In the NR case this also happens by inserting $2m_0$ or $2m$ instead of m_0, where m is the reduced mass.

II. BASIC EQUATIONS

First the QM dispersions of H_1 and H_2 are

$$\delta H_1(x) = m_0/x\,[2\sqrt{1+x^2} - \alpha_0 - g_0 \exp(-\gamma d_0 x)] , \quad (5)$$

and

$$\delta H_2(x) = m_0/x \left(\frac{1}{x} - \alpha_0 - g_0 \exp(-\gamma d_0 x) \right) , \quad (6)$$

where

$$x = r/l_1, \quad l_1 = \hbar d_0/m_0, \quad \alpha = \alpha_0 d_0, \quad g = g_0 d_0, \quad \mu = m_0 \gamma .$$

Next the generalized virial theorem[12] yields the algebraic equations

$$\lambda = f_1(u) = (u^2 + \gamma^2 d_0^2)^{1/2}[q + f(u)] \quad (7)$$

and

$$\lambda = f_2(u) = u[q + f(u)] , \quad (8)$$

in which $u = \gamma d_0 x$, $q = \alpha_0/g_0$, $u \in (0,\infty)$, whereas $\lambda = 2d_0\gamma/g_0$ denotes the dimensionless screening parameter. One also has

$$f(u) = (u+1)\exp(-u) , \quad (9)$$

which decreases with u, so that $f(u) \in (1,0)$ for $u \in (0,\infty)$. Equations (7) and (8) give the location of the minima of $\delta H_1(x)$ and $\delta H_2(x)$, insofar as the concavity conditions

$$\lambda > \tilde{f}_1(u) = (u^2+\gamma^2 d_0^2)^{3/2}\exp(-u) \quad (10)$$

and

$$\lambda > \tilde{f}_2(u) = u^3\exp(-u) \quad (11)$$

are fulfilled, respectively. Now we shall prove that Eqs. (7)–(11), as well as their by-products, though very simple, actually express an efficient and general investigation of the GSE problem.

III. THE COULOMB PROBLEM

Let us ignore the Yukawa potential at the beginning. Then Eqs. (1), (7), and (10) produce the two-particle GSE,

$$\mathscr{E}_0 = 2m_0[1-(\alpha_0^2/4)]^{1/2}, \quad (12)$$

in which the inequality

$$\alpha_0 < \alpha_c = 2 \quad (13)$$

has the meaning of the Coulomb stability threshold. Equation (13) is simply an inequality by-product of Eq. (7). Now one sees immediately that the single-particle counterpart of Eq. (12) reproduces exactly the well-known GSE $\mathscr{E}_0' = m_0(1-\alpha^2)^{1/2}$ of the R hydrogen atom[17] if $d_0 = 1$. Moreover, Eq. (13) is identical to the Coulomb stability threshold $\alpha < 2$ (Ref. 18) established for two interacting massless spin-$\frac{1}{2}$ particles, if $d_0 = 1$ also. In this respect proofs have been given that Eq. (13) is also valid within the zero-mass limit.[15] These agreements enable us to say that the present approach effectively yields the GSE's for two interacting R-spin-$\frac{1}{2}$ particles if one sets $d_0 = 1$, thereby relying on the dominant Coulomb-type behavior of the potential near the origin. For the sake of generality we shall maintain, however, the inclusion of d_0. Of course, Eqs. (1), (8), and (11) yield the GSE

$$E_0 = -m_0\alpha_0^2/4, \quad (14)$$

which is the NR limit of Eq. (12). The concavity condition is $\alpha_0 > 0$ in both cases. However, $\alpha_0 > 0$ comes up in terms of the virial equation, so that the concavity condition is superfluous with respect to the Coulomb problem.

Further, we shall use this opportunity to analyze the more general R superposition,

$$H_1^*(r,p) = -(\alpha\hbar/r) + \{p^2+[m_0-(\beta\hbar/r)]^2\}^{1/2}, \quad (15)$$

where $-\beta\hbar/r\,(\beta=\beta_0 d_0)$ denotes the scalar Coulomb potential. First the virial equation reads

$$1/x = [\beta_0/(1+\beta_0^2)][1+(\alpha_0/\beta_0)(1+\beta_0^2-\alpha_0^2)^{-1/2}], \quad (16)$$

which is meaningful only if $1+\beta_0^2 > \alpha_0^2$. Next, it follows that the region $\alpha_0 < 0$ and $\beta_0 < 0$ of the (α_0, β_0) plane is forbidden. Note that the concavity condition is fulfilled automatically in terms of Eq. (16), which agrees with the similar conjecture mentioned above. So one obtains the GSE

$$\mathscr{E}_0^* = [m_0/1+\beta_0^2][(1+\beta_0^2-\alpha_0^2)^{1/2}-\alpha_0\beta_0], \quad (17)$$

if

$$\alpha_0^2 < 1+\beta_0^2, \quad \alpha_0 > 0, \quad \beta_0 > 0,$$
$$\alpha_0^2 < \beta_0^2 < 1+\beta_0^2, \quad \alpha_0 < 0, \quad \beta_0 > 0, \quad (18)$$
$$\beta_0^2 < \alpha_0^2 < 1+\beta_0^2, \quad \alpha_0 > 0, \quad \beta_0 < 0.$$

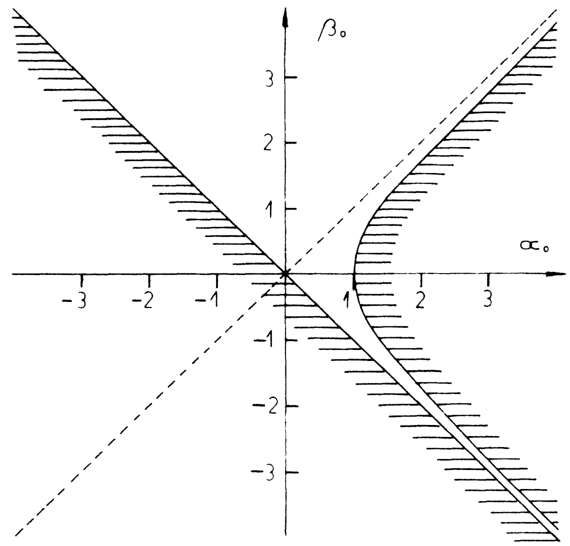

FIG. 1. Phase-structure diagram characterizing the Hamiltonian (15). The GSE (17) can be defined only outside the hatched domains, i.e., to the left of the right-hand side hyperbole branch $\alpha_0^2 = 1+\beta_0^2$, as well as above the second bisectrix $\alpha_0 = -\beta_0$.

Equation (18) establishes the phase structure characterizing Eq. (15), as shown in Fig. 1. One sees that $\mathscr{E}_0^* \in (-m_0, m_0)$, in contradistinction to $\mathscr{E}_0' \in (0, m_0)$. In addition, one has $0 < \mathscr{E}_0^* < m_0$ if $\alpha_0 < 1$, whereas $-m_0 < \mathscr{E}_0^* < 0$ if $\alpha_0 > 1$. So far $\alpha_0 > 0$ and $\beta_0 > 0$. Furthermore, $0 < \mathscr{E}_0^* < m_0$ for $\mathrm{sgn}\alpha_0 = -\mathrm{sgn}\beta_0$. So $\mathscr{E}_0^* \to -m_0$ for $\alpha_0 \to \infty$ and $\beta_0 \to \infty$, while $\mathscr{E}_0^* = m_0$ for $\alpha_0 = \beta_0 = 0$, as well as on the second bisectrix.

IV. THE NONRELATIVISTIC YUKAWA POTENTIAL

For the next step let us set $\alpha_0 = 0$. Considering the NR case, one would then have the virial equation

$$\lambda = g_2(u) = uf(u). \quad (19)$$

One realizes that $g_2(u)$ is centered around its maximum point

$$u = v_0 = (1+\sqrt{5})/2 \cong 1.6180, \quad (20)$$

so that $g_2(0) = g_2(\infty) = 0$, as shown in Fig. 2(a). Then Eq. (19) exhibits positive u roots only if

$$\lambda < \lambda_c^{(2)} = g_2(v_0) \cong 0.8399. \quad (21)$$

This shows the existence of the critical screening parameter $\lambda_c^{(2)}$. We might remark that within the single-particle case $\lambda = \lambda' = \gamma d_0/g_0$. Thus Eq. (21) compares reasonably well with the critical evaluations $\lambda' < 1.19$ (Ref. 9) and $\lambda' < 1.19060$ (Ref. 5) established previously on this subject. Next, the concavity condition reads $u < v_0$, so that the GSE is produced by the smaller root of Eq. (19); see Fig. 2(b). On the other hand, Eq. (19) also leads to $u > v_0'$, so that

$$u \in (v_0', v_0), \quad (22)$$

where

$$v_0' = \tfrac{1}{2}[(1+4\lambda)^{1/2}-1]. \quad (23)$$

These results enable us to define uniquely the GSE as

$$E = \delta H_2(u) = m_0\gamma^2 d_0^2(u-1)/u^2(u+1), \quad (24)$$

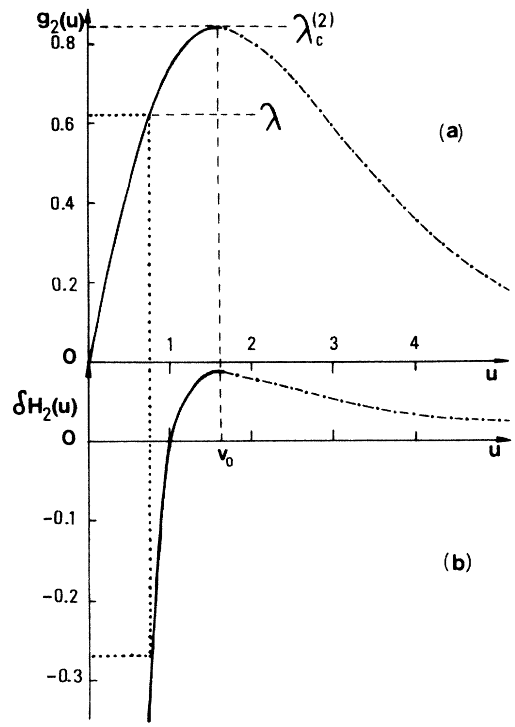

FIG. 2. The u dependence of (a) $g_2(u)$ and (b) $\delta H_2(u)$. The solid curves show that both $g_2(u)$ and $\delta H_2(u)$ increase with u if $u < v_0$. Along the dot-dashed curves the concavity condition is not fulfilled. Here the GSE is measured in $\gamma^2 d_0^2 m_0$ units. The dotted lines show how one obtains the GSE by starting from a given $\lambda < \lambda_c^{(2)}$ value, and vice versa.

where u is subject to Eqs. (19) and (22). Further, one has the constraints

$$\delta H_2(v_0') < E < \delta H_2(v_0) \cong 0.0901 m_0 \gamma^2 d_0^2 \ , \tag{25}$$

in which $\delta H_2(v_0') < 0$, as $\lambda < 2$. We note the appearance of positive-energy excitations for $1 < u < v_0$ and mention that the concavity domain $u < v_0$ is also the exclusive u region in which both $g_2(u)$ and $\delta H_2(u)$ increase with u, and conversely.

V. THE RELATIVISTIC YUKAWA POTENTIAL

Within the R case the virial theorem reads

$$\lambda = g_1(u) = (u^2 + \gamma^2 d_0^2)^{1/2} f(u) \ . \tag{26}$$

Combining Eqs. (26) and (10) one finds

$$\lambda^2 < F(u) = (1+u)^3 \exp(-2u) \ , \tag{27}$$

which in turn produces necessarily the critical screening parameter

$$\lambda < \lambda_c^{(1)} = \sqrt{F(0.5)} = (3/2)^{3/2} \exp(-0.5) \cong 1.1142 \ . \tag{28}$$

Above $F(u)$ is centered around its maximum point $u = 0.5$, whereas $F(0) = 1$ and $F(\infty) = 0$. The present concavity condition is $u^2 + \gamma^2 d_0^2 < u + 1$, which involves the critical mass quotient

$$\gamma d_0 < \tilde{\gamma}_c^{(1)} = \sqrt{5}/2 \cong 1.1180 \ , \tag{29}$$

as well as the admissible u interval

$$u \in (u_-, u_+) \ , \tag{30}$$

in which

$$u_\pm = \tfrac{1}{2} \pm (\tfrac{5}{4} - \gamma^2 d_0^2)^{1/2} \ . \tag{31}$$

Under such conditions Eq. (26) exhibits u roots belonging to the concavity interval (30) if

$$\begin{aligned} &g_c^{(-)} > g_0 > g_c^{(+)} > 2, \quad \tilde{\gamma}_c^{(1)} > \gamma d_0 > \gamma_1 \ , \\ &g_c^{(-)} > g_0 > g_c^{(+)}, \quad \gamma_1 > \gamma d_0 > 1 \ , \\ &2 > g_0 > g_c^{(+)}, \quad \gamma d_0 < 1 \ , \end{aligned} \tag{32}$$

in which $\gamma_1 \cong 1.1024$. These inequalities establish the increasing branches of $g_1(u)$, as shown in Fig. 3. Note that $\lambda \gtrless \gamma d_0$ reads $g_0 \lesseqgtr 2$, whereas $g_c^{(+)} < 2 < g_c^{(-)}$ for $\gamma_1 > \gamma d_0 > 1$. In Eq. (32)

$$g_c^{(\pm)} = g_c^{(+)}(\gamma d_0) = 2\gamma d_0 (1 + u_\pm)^{-3/2} \exp(u_\pm) \ . \tag{33}$$

Equation (32) establishes the phase-structure diagram in the $(g_0, \gamma d_0)$ plane, characterizing the R-Yukawa-Hamiltonian. The above results lead to the GSE

$$\mathscr{E} = \delta H_1(u) = 2m_0(u^2 + u + \gamma^2 d_0^2)/(u+1)(u^2 + \gamma^2 d_0^2)^{1/2} \ , \tag{34}$$

where u is subject to Eqs. (26) and (30). In consequence

$$\begin{aligned} &2\gamma d_0 m_0 < \mathscr{E} < \delta H_1(u_+), \quad \gamma d_0 < 1 \ , \\ &\delta H_1(u_-) < \mathscr{E} < \delta H_1(u_+), \quad \gamma d_0 > 1 \ , \end{aligned} \tag{35}$$

where $\delta H_1(0) = 2\gamma d_0 m_0$. In agreement with Eq. (30), both $g_1(u)$ and $\delta H_1(u)$ increase simultaneously with u for $u \in (0, u_+)$ if $\gamma d_0 < 1$, as well as for $u \in (u_-, u_+)$ if $\gamma d_0 > 1$. Above $\delta H_1(u_+) > 2m_0$, whereas

$$\begin{aligned} &\delta H_1(u_-) < 2\gamma d_0 m_0, \quad 1 < \gamma d_0 < \gamma_1' \ , \\ &\delta H_1(u_-) > 2\gamma d_0 m_0, \quad \gamma_c^{(1)} > \gamma d_0 > \gamma_1' \ , \end{aligned} \tag{36}$$

in which $\gamma_1' \cong 1.0765$ (see Fig. 4). We note that $\delta H_1(u_-) > 2m_0$ for $\gamma d_0 > 1$. If $\gamma d_0 < 1$, one has $\delta H_1(u) \leq 2m_0$, insofar as $u \leq u_+' = (1 - \gamma^2 d_0^2)^{1/2}$. This latter case is compatible with the NR limit of zero-energy binding. In the other cases positive-energy excitations would also be involved. At this end we also note that the complex u roots characterizing Eqs. (7) and (8) can also be interpreted in terms of the possible onset of underlying resonances.[19]

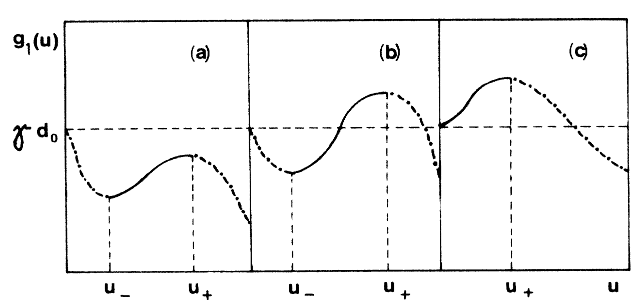

FIG. 3. Plots of $g_1(u)$ vs u for (a) $\tilde{\gamma}_c^{(1)} > \gamma d_0 > \gamma_1$, (b) $\gamma_1 > \gamma d_0 > 1$, and (c) $\gamma d_0 < 1$. The solid curves are responsible for the GSE's. Along the dot-dashed curves $g_1(u)$ decreases with u, so that the concavity condition is not fulfilled.

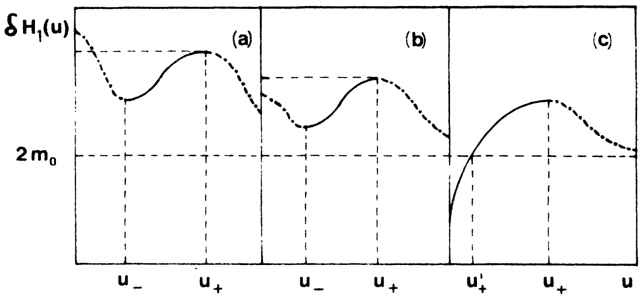

FIG. 4. Plots of $\delta H_1(u)$ vs u for (a) $\tilde{\gamma}_c^{(1)} > \gamma d_0 > \gamma_1'$, (b) $\gamma_1' > \gamma d_0 > 1$, and (c) $\gamma d_0 < 1$. One sees that (a) $\delta H_1(0) > \delta H_1(u_+)$ and (b) $\delta H_1(0) < \delta H_1(u_+)$. The solid curves are involved exclusively in each case.

VI. CONCLUSIONS

The above results show that the quasiclassical approach to the virial theorem can be used satisfactorily in order to establish in a simple manner reasonable estimates of GSE's and of stability thresholds. The main capability of the present approach concerns, however, the possibility of establishing relevant analytic forms and typical structural properties characterizing the estimates mentioned above. Such evaluations are then able to reproduce the actual results up to suitable values of the $d_0 \sim 1$ parameter. Phase-structure diagrams like those exhibited by Eqs. (18) and (32) are also of real interest. Of course one has a valuable motivation for using such a quasiclassical approach with respect to more complicated potentials, momentum-dependent ones included, which are hardly tractable with the help of standard methods. The Coulomb potential turns out to be a special limiting case, as the GSE is reproduced exactly if $d_0 = 1$. This choice also expresses the self-consistent evaluation of the underlying phase-space quantum. In general, the present quasiclassical approach, though expressing an efficient qualitative method, is able to produce reasonable approximations, like those obtained for the Yukawa potential. This conjecture agrees with the usual Wentzel-Kramers-Brillouin approach, which is subject to similar limitations. In the present case such limitations come from the underlying quasiclassical non-Hermitian limits of the momentum powers.[16] For non-Coulomb potentials some further refinements would then be desirable. Comparisons with available data could also be used in order to refine the d_0 choice.

Finally, let us say a few remarks concerning the superposition (3). Proceeding in the same manner leads to the GSE's

$$E_s = \delta H_2^{(s)}(u) = -\gamma d_0 \alpha_0 m_0 \frac{2u^2 - \lambda_0 u + \lambda_0}{2u^2(u+1)} , \tag{37}$$

where $\lambda_0 = 2\gamma d_0/\alpha_0$, and

$$\mathscr{E}_s = \delta H_1^{(s)}(u) = m_0 \left[\frac{2(u^2+\gamma^2 d_0^2)+2u}{(u+1)(u^2+\gamma^2 d_0^2)^{1/2}} - \frac{\alpha_0 \gamma d_0}{u+1} \right] , \tag{38}$$

in the NR and R cases, respectively. The corresponding concavity conditions mean that u should be restricted only to the mutually identical regions in which, similarly as before, both $f_2(u)$ and $\delta H_2^{(s)}(u)$, as well as $f_1(u)$ and $\delta H_1^{(s)}(u)$ increase with u. Then u is subject only to Eqs. (8) and (7), respectively. Some additional peculiarities, such as bifurcations toward two minima, should also be observed.[20] We also note that E_s and $\mathscr{E}_s$ are located below the corresponding Coulomb GSE's (14) and (12), as one might expect.

Note added in proof. Using energy upper bounds for hydrogenlike problems, Eq. (21) has also been obtained by R. L. Hall, Phys. Rev. A 32, 14 (1985), via his Eq. (4.11). It should be mentioned that, within a suitable d_0 choice, our Eq. (1) reproduces the right-hand side of his Eq. (1.8).

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[16]More definitely, momentum powers should be defined in terms of dilations. So, the usual square-momentum operator $\hat{p}^2 = -\hbar^2\Delta$ is subject to the expansion $\hat{p}^2 = (1/r^2)(\hat{a}^2 + i\hbar\hat{a})$. This leads to the quasiclassical limit $\hat{P}^2 \equiv \lim_{\hbar\to 0}\hat{p}^2 = (1/r^2)\hat{a}^2$, while $\lim_{\hbar\to 0}(1/i\hbar) \times [\hat{P}^2, r] = 2\hat{P}$, as one might expect. The main point is that this time one has $\hat{P}^2(1/r) = -(\hbar^2/r^2)(1/r)$ instead of $\hat{p}^2(1/r) = 4\pi\hbar^2\delta(\mathbf{x})$, thereby accomplishing a "non-Hermitian" regularization of the undesirable $\delta(\mathbf{x})$ singularity; see Ref. 15.

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