New Method for Calculating Binding Energies in Quantum Mechanics and Quantum Field Theories

G. Gat[1] and B. Rosenstein[2]
[1] *Physics Department, University of Maryland, College Park, Maryland 20742*
[2] *Institute of Physics, Academia Sinica, Taipei, 11529, Taiwan*
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We propose a systematic perturbative method for calculating the binding energy of threshold bound states—states which exist for arbitrary small coupling. The starting point is a (regularized) free theory. Explicit calculations are performed for quantum mechanics with arbitrary short-range potential in 1D and various $(1+1)$-dimensional quantum field theories. We check the method by comparing the results with exact formulas available in solvable models.

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Threshold bound states.—The study of bound state spectra is one of the most interesting and difficult problems in quantum mechanics and especially in quantum field theory. The main difficulty is that the problem is essentially "nonperturbative." Other quantities, like scattering amplitudes, are usually calculated perturbatively for weak coupling. However, the study of even the simplest bound states, like the hydrogen atom, requires the use of special methods.

In quantum mechanics in order to study a potential it is approximated by one of the solvable potentials, i.e., those for which the spectrum is known exactly. The deviations are then taken into account systematically in perturbation theory. In quantum field theory the available approximation schemes [1] are usually very complicated and by no means systematic. Even for weakly coupled theories like QED the calculation should be considered an "art" [1]. The standard wisdom in quantum mechanics as well as quantum field theory is that the perturbation theory around free theory is inapplicable for the study of bound states [2]. If all the interactions are considered a small perturbation, to any *finite* order in perturbation theory there are no poles in the scattering matrix. It is easy to understand the reason behind this conclusion by considering the bound state spectrum of a square-well potential in three dimensions. As the depth of the well decreases the bound states are "swallowed" one by one by the continuum. Beyond some critical depth there are no bound states left in the spectrum. Clearly, weak coupling perturbation theory has nothing to do with such bound states. There is, however, a class of bound states which exist for any value of the coupling constant no matter how small. An example of such "threshold" bound states is the hydrogen atom $E_n = \frac{\alpha^2}{2n^2}$. When the fine structure constant $\alpha \to 0$, the spectrum becomes denser but no bound state is lost in the continuum. For such bound states the above conclusion is not warranted.

Threshold bound states happen to be quite abundant in quantum mechanics and quantum field theory. They include the lowest bound state of essentially any short-range potential in 1D and 2D quantum mechanics and in 1+1 and 2+1 quantum field theories, all the bound states of QED, and even hadrons in QCD. Perturbation theory does "know" about such states. One encounters threshold or on-shell infrared singularities in scattering amplitudes when momenta approach the threshold.

In this Letter we reconsider the use of weak coupling perturbation theory [3] for the calculation of binding energies of a large class of such states.

First, we limit ourselves to the case when the binding energy E not only approaches zero as the coupling $\alpha \to 0$ but is also an analytic function of α. General theorems (and simply experience with exactly solvable models) tell us that this class includes (i) the lowest bound state of all the potentials in 1D that decay at large distances faster than a power, (ii) most of the bound states for potentials in 3D that asymptotically fall as $1/r$ at large distances, and (iii) many bound states in quantum field theories (QFT) in 1+1 dimensions.

For short-range potentials $\alpha V(x)$ in 1D Simon proved that the energy of the lowest bound state is analytic in α [4] and derived the following expansion:

$$E(\alpha) = -\frac{1}{2}\alpha^2 \left(\int_x V(x)\right)^2 - \alpha^3 \int_x \int_y V(x)|x-y|V(y) \int_z V(z) + O(\alpha^4)\,. \tag{1}$$

Well-known solvable examples include [5] the δ potential $V(x) = -\alpha\delta(x)$ for which $E_0 = -\alpha^2/2$, the square well $V(x) = -\alpha\theta(a-|x|)$ $(E_0 = -2ma\alpha^2)$, and the Pöschel-Teller potential $V(x) = -\frac{\alpha}{\cosh(x)^2}$ $[E_0 = -\frac{2\alpha^2}{m} + O(\alpha^3)]$. For 3D potentials decreasing as $1/r$ at large distances, most bound states are threshold and analytic. During the last decade since the solution of the Thirring model many exact results for so-called solvable $(1+1)$-dimensional quantum field theories became available. When one looks at the coupling dependence of the threshold bound states in these mod-

els the analyticity becomes evident. For example, in the Thirring model

$$\mathcal{L} = \bar{\psi}(i\partial\!\!\!/ - m)\psi + \tfrac{1}{2}g(\bar{\psi}\gamma_\mu\psi)^2 \tag{2}$$

the mass of the bound state meson (the "sine-Gordon" particle) is

$$M_2 = 2M_f \sin\left(\frac{\pi}{2(1+\frac{2g}{\pi})}\right) = M_f\left(2 - g^2 + \frac{4g^2}{\pi} + \cdots\right), \tag{3}$$

where M_f is the elementary fermion mass. So the case of analytic threshold bound states is by no means pathological or exceptional.

For these states the situation is rather peculiar. We do know, on one hand, that the binding energy has an (even convergent) expansion in the coupling α, but, on the other hand, no apparent poles appear in the expansion of the S matrix to any finite order in perturbation theory. A natural question arises: Why not calculate binding energies directly? One does not have to calculate the scattering matrix first and then look for poles in it. These two operations are nonperturbative. We show that the direct perturbation theory for bound states around the free theory (done with some care) does, in fact, work.

To demonstrate how the procedure works, we start with a somewhat detailed calculation in 1D quantum mechanics (for arbitrary short-range potential). Then two (1 + 1)-dimensional quantum field theories are considered up to third order in α: the Thirring model and the polynomial interaction. The Thirring model is a solvable one, so we can confront the results against known binding energies.

Quantum mechanics.—A straightforward calculation of binding energy in standard perturbation theory starting from the free theory $H = -\frac{1}{2}\frac{\partial^2}{\partial x^2}$ is not possible due to infrared on-shell divergencies. We therefore first regularize the infrared (on-shell) divergencies by adding a solvable potential $\beta V_{\rm reg}(x)$ which has similar threshold bound state structure. The regularized theory is then perturbed by the interaction $\alpha V(x)$ to some finite order in α. At the end of the calculation the regulating potential is taken to zero (i.e, we take the limit when its coefficient β goes to zero). We choose $V_{\rm reg}(x) = -\delta(x)$. The spectrum of the unperturbed regularized Hamiltonian $H_0(\beta)$ consists of one bound state $|0\rangle = \sqrt{\beta}e^{-\beta|x|}$ and the continuum, $|p\rangle_{\rm even} = \frac{\sqrt{2}}{p-i\beta}[p\cos(px) - \beta\sin(p|x|)]$ and $|p\rangle_{\rm odd} = \sqrt{2}\sin(px)$. The corresponding energies are $E_0 = -\frac{\beta^2}{2}$ and $E_p = \frac{p^2}{2}$. The first-order correction to the energy is [we take the symmetric potential $V(x) = V(-x)$]

$$E_1(\beta) = \langle 0|V|0\rangle = \alpha\beta\int dx V(x)e^{-2\beta|x|} \xrightarrow{\beta\to 0} 0. \tag{4}$$

It turns out that the limit $\beta \to 0$ is conveniently taken by expanding in β. The second-order correction is given by

$$\Delta E_2 = \int \frac{dp}{2\pi}\frac{|\langle 0|v|p\rangle_{\rm even}|^2}{E_0 - E_p} = -\frac{2\beta\alpha^2}{\pi}\int_{x,y}\int_p e^{-\beta(|x|+|y|)}\frac{V(x)V(y)}{(p^2+\beta^2)^2}\left[p^2\cos(px)\cos(py) - p\beta\sin(|x|+|y|) + \beta^2\sin(px)\sin(py)\right]. \tag{5}$$

In addition to factors of β coming from the bound state normalization there are factors of $1/\beta$ coming from integration over momenta around the $p = 0$ threshold. In other regions of the integration one is allowed to expand the integrand in β. Performing the p integration we get a finite result,

$$\Delta E_2 = -\frac{\alpha^2\beta}{\pi}\int_{x,y}\int_p V(x)V(y)\frac{p^2\{\cos[p(x+y)] + \cos[p(x-y)]\}}{(p^2+\beta^2)^2} + O(\beta) \xrightarrow{\beta\to 0} -\frac{\alpha^2}{2}\left[\int_x V(x)\right]^2, \tag{6}$$

which coincides with the first term in the exact expansion of Simon Eq. (1). Analogously the third-order term is

$$\Delta E_3 = \int_{p,q}\frac{1}{(2\pi)^2}\frac{\langle 0|V|p\rangle\langle p|V|q\rangle\langle q|V|0\rangle}{(E_0 - E_p)(E_0 - E_q)} - \langle 0|V|0\rangle\int_p \frac{1}{2\pi}\frac{|\langle 0|V|p\rangle|^2}{(E_0 - E_p)^2} \equiv \alpha^3(E_3^a - E_3^b). \tag{7}$$

The expressions for E_3^a and E_3^b have the following Laurent expansion in β:

$$E_3^a = \frac{1}{4\beta}\left[\int_x V(x)\right]^3 - \int_x V(x)\left[\int_x |x|V(x)\right]^2 - \int_x V(x)\int_{x,y} V(x)|x-y|V(y) + O(\beta),$$
$$E_3^b = \frac{1}{4\beta}\left[\int V(x)\right]^2 - \frac{1}{2}\int_{x,y}(|x|+|y|)V(x)V(y) + O(\beta). \tag{8}$$

We observe that the $1/\beta$ term in E_3^a cancels that in E_3^b. The finite contribution

$$\lim_{\beta\to 0}\Delta E_3 = -\alpha^3\int_x V(x)\int_{x,y} V(x)|x-y|V(y) \qquad (9)$$

again agrees with the exact formula of Simon.

Our choice of regulator is quite arbitrary. One could perform the same calculation with any other attractive short-range potential. The only requirement is that the regularized Hamiltonian $H_0(\beta)$ has a bound state with the same quantum numbers as the one for which the binding energy is calculated. The regulator "fixes" the unperturbed state roughly at the location of the bound state. The calculation itself is *much simpler* than that in standard perturbation theory around a nontrivial interaction Hamiltonian. Although we are expanding around a nontrivial regularized model, the use of the Laurent expansion simplifies the calculation of integrals considerably.

Quantum field theory.—In order to be able to compare with a known spectrum we start with a solvable QFT: the Thirring model, Eq. (2). For weak coupling it is known that there is only one fermion-antifermion threshold bound state with energy given in Eq. (3) [6]. Now we have to regularize the free theory by adding interaction. Unlike the situation in quantum mechanics, in relativistic quantum field theory a covariant interaction term like $(\bar\psi\psi)^2$ necessarily mixes sectors of the Hilbert with a different number of particles. The regularized Hamiltonian $H_0(\beta)$ then becomes a nontrivial quantum field theory and is useless for our purposes. However, we have already seen that the only purpose of introducing a regulator is to "fix" the mesonic bound state. Therefore one can choose as a regulator an interaction which is restricted to the two-particle sector only. This, of course, breaks Lorentz invariance which is restored in the $\beta\to 0$ limit.

The simplest attractive interaction of this kind is the contact one:

$$H_0(\beta) = \sum_p \omega(p)a_p^\dagger a_p + \beta\mathcal{P}\sum_{p_1,p_2,p_3} a_{p_1}^\dagger a_{p_2}^\dagger a_{p_3}a_{-p_1-p_2-p_3}\,, \qquad (10)$$

where $\omega(p)\equiv\sqrt{p^2+m^2}$ and $\mathcal{P}$ is a projection operator on the two-particle sector. This Hamiltonian can be easily diagonalized. Acting with Hamiltonian Eq. (10) on two-particle states in the center-of-mass frame of reference $|\Psi_b\rangle \equiv \int_{p_1,p_2}\delta(P)\Psi_b(p)a_{p_1}^\dagger a_{p_2}^\dagger|0\rangle$ ($p=\frac{p_1-p_2}{2}$ and $P=p_1+p_2$) one obtains the following Schrödinger equation:

$$2\omega(p)\Psi(p) - \beta\int_{-M}^{M}\frac{dk}{2\pi}\Psi(k) = E\Psi(p)\,. \qquad (11)$$

So essentially we get a δ potential with a relativistic dispersion relation. Since the integral in this equation diverges, we introduced a cutoff M. The effect of introducing the cutoff is that the δ interaction is smeared. The divergence can be absorbed in the redefinition of the coupling β, i.e., $\tilde\beta = \frac{\beta}{1-\beta M/2\pi}$ (in the following we drop the tilde).

Solving the equation one finds one bound state whose wave function is

$$\Psi(p)_b = \frac{\sqrt{N}}{2w(p)-2m+\Delta}\,, \qquad (12)$$

where Δ the binding energy is defined by

$$\frac{1}{\beta} = \int_{-M}^{M}\frac{dp}{2\pi}\frac{1}{2\omega(p)-2m+\Delta}\,. \qquad (13)$$

It has an expansion $\Delta = \frac{\beta^2}{4}[1-\frac{\beta}{\pi}+O(\beta^2)]$. The normalization constant N has the following expansion: $N = \frac{\beta^3}{4}[1-\frac{\beta}{\pi}+O(\beta^2)]$. The scattering solutions are

$$\Psi(p)_k = 2\pi\delta(p-k) + \frac{\beta}{[2\omega(p)-2\omega(k)+i\epsilon]}\frac{2\beta k}{[2k-i\beta\omega(k)]}. \qquad (14)$$

The leading-order contribution in $V = g/2(\bar\psi\gamma_\mu\psi)^2$ vanishes:

$$\Delta E_1 = \langle\Psi_b|V|\Psi_b\rangle = \int_{p,q}\Psi_b(p)\Psi_b(q)\langle p,-p|V|q,-q\rangle = g\beta + O(\beta^2)\overset{\beta\to 0}{\longrightarrow} 0. \qquad (15)$$

The first nonvanishing contribution appears in second order. To this order one should, in principle, take into account all the virtual transitions from the two-particle sector to the two- (continuum as well as bound state), four-, and six-particle sectors: $\Delta E_2 = E_{2\to 0\to 2} + E_{2\to 2\to 2} + E_{2\to 4\to 2} + E_{2\to 6\to 2}$. The "elastic" contribution is

$$E_{2\to 2\to 2} = \int\frac{dp}{2\pi}\frac{|\langle\Psi_b|V|\Psi(p)_k\rangle|^2}{E_0-2\omega(p)}\,. \qquad (16)$$

The factors of β coming from the bound state normalization will be compensated by $1/\beta$ terms coming from the integration region close to the threshold ($p^2=4m^2$). The remaining $2\to 2\to 2$ contributions are

$$E_{2\to 2\to 2} = \frac{g^2}{4}NX^2I\overset{\beta\to 0}{\longrightarrow} -g^2\,, \qquad (17)$$

where

$$X = \int_0^\infty\frac{dp}{\pi}\frac{2}{\omega(p)[\omega(p)-2m+\Delta]} = \frac{2}{\beta}+O(\beta)\,,$$
$$I = \int_0^\infty\frac{dp}{\pi}\frac{16p^2}{\omega(p)^2[4p^2+\beta^2\omega(p)^2][2\omega(p)-2m+\Delta]} = -\frac{2}{\beta}+\frac{3}{2\pi}+O(\beta)\,. \qquad (18)$$

Equation (17) coincides with the first term in the expansion of the exact formula for the binding energy of the lowest bound state in the Thirring model, Eq. (3). It is easy to see, by simply counting powers of β, that only transitions within the two-particle sector survive in the limit $\beta \to 0$. The reason for that is the following. The integrals in the other contributions, for example,

$$E_{2\to4\to2} = \int \frac{1}{(2\pi)^4}\delta(p_1+p_2+p_3+p_4)\frac{|\langle\Psi_b|V|p_1,p_2,p_3,p_4\rangle|^2}{E_0-\omega(p_1)-\omega(p_2)-\omega(p_3)-\omega(p_4)}\,, \tag{19}$$

have no singularities so that no factor of $1/\beta$ can be produced. This is due to the fact that there is a finite energy gap for these virtual processes. The contribution from these processes will therefore vanish in the limit $\beta \to 0$.

In the third order there are still no contributions to processes connecting the two-particle sector with higher sectors [7]. Performing the calculation we get

$$\Delta E_3 = \frac{g^3}{8}\left[NX^2I^2 + N^2X^4\frac{\partial I}{\partial\Delta}\right] \xrightarrow{\beta\to0} g^3\frac{4}{\pi} \tag{20}$$

which again agrees with Eq. (3).

A similar calculation for the (nonsolvable) polynomial interaction

$$\mathcal{L} = \tfrac{1}{2}\partial_\mu\phi\partial^\mu\phi - \tfrac{1}{2}m^2\phi^2 + \lambda\phi^4 - \eta\phi^6 \tag{21}$$

gives

$$M_2 = 2M - \frac{9}{4}\frac{g^2}{M^3} + \frac{27}{2\pi}\frac{g^3}{M^5} + O(g^4)\,, \tag{22}$$

where g is the renormalized four-coupling. The first term agrees with previous calculations of [8] while the second term is new. For comparison we include the expansion of the variational calculation of the two-particle bound state of Ref. [9],

$$M_2 = 2M - \frac{9g^2}{4M^3} + \frac{27}{8}\left(\frac{2}{\pi}+1\right)\frac{g^3}{M^5}\,.$$

The g^3 coefficient is $\sim 20\%$ off.

Conclusion.—The method proposed here is systematic and straightforward. All the integrals involved can be found in tables, so that no numerical calculation is required. In contrast, the Bethe-Salpeter scheme starts by replacing the leading-order Bethe-Salpeter equation by a solvable (usually nonrelativistic) integral equation. One then performs a double "expansion." The kernel is corrected perturbatively and in addition one should correct the initial approximation to the leading order.

To summarize, the direct calculation of binding energies of threshold bound states, using regularized perturbation theory, was shown to work for quantum mechanical problems of arbitrary short-range potentials and for massive quantum field theories in 1+1 dimensions. Generalizations to higher dimensions are straightforward.

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[1] C. Itzykson and J.B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).

[2] A.I. Baz, Ya.B. Zeldovich, and A.M. Perelomov, *Scattering, Reactions and Decays in Nonrelativistic Quantum Mechanics* (Nauka, Moscow, 1966).

[3] For a previous (unsuccessful) attempt, see E.P. Wigner, Phys. Rev. **94**, 77 (1954); R.E. Trees, Phys. Rev. **102**, 1553 (1956).

[4] B. Simon, Ann. Phys. (N.Y.) **97**, 279 (1976); **108**, 69 (1977).

[5] S. Flügge, *Practical Quantum Mechanics* (Springer-Verlag, Berlin, 1970), Vol. I; M. Znojil, J. Phys. A **20**, 1751 (1987).

[6] A.B. Zamolodchikov and A.B. Zamolodchikov, Ann. Phys. (N.Y.) **120**, 253 (1979).

[7] There will be contributions from such transitions in higher orders since the expression for the shift will contain contributions which correspond to hopping a few times within the two-particle sector. In diagramatic language these correspond to subleading infrared divergencies occurring in Feynman diagrams of this process; see R.J. Eden, P.V. Landshoff, D.I. Olive, and J.C. Polkinghorne, *The Analytic S-Matrix* (Cambridge Univ. Press, Cambridge, 1966), p. 57. This gives enough factors of $1/\beta$ to allow the jump to other sectors.

[8] J. Dimock and J.P. Eckmann, Commun. Math. Phys. **51**, 41 (1976); Ann. Phys. (N.Y.) **103**, 289 (1977).

[9] P.M. Stevenson, Phys. Rev. D **33**, 2305 (1986); J. Darewych, M. Horbatsch, and R. Koniuk, Phys. Rev. Lett. **54**, 2188 (1985).