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Spin Polarizabilities on the Lattice

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Spin polarizabilities provide information on the internal structure of hadrons in the presence of weak external electromagnetic fields, and are actively studied by Compton scattering experiments. They provide finer detail than the regular polarizabilities since they require space and time-varying fields. Using an effective action in the weak field limit, we have identified methods to isolate each of the physical quantities $(\mu, \alpha, \beta, \gamma_{E1}, \gamma_{M1}, \gamma_{E2}, \gamma_{M2})$ for spin-1/2 hadrons, both neutral and charged. We also perform a lattice QCD simulation to investigate the feasibility of the effective action approach.

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1. Introduction

The interaction of a spin-1/2 hadron with a weak external electromagnetic field can be described by an effective, non-relativistic quantum mechanical (QM) action in Euclidean space as [1]

$$S_{QM} = \int d^4x\, L_{QM}, \tag{1.1}$$

where the effective QM Lagrangian is given by

$$\begin{aligned} L_{QM} \;=\; & \psi^\dagger(x,t)\left[\left(\frac{\partial}{\partial t}\right) + (-i\vec{\nabla} - q\vec{A})^2 - \mu\vec{\sigma}\cdot\vec{B} + \frac{1}{2}\alpha\vec{E}^2 - \frac{1}{2}\beta\vec{B}^2 \right.\\ & \left. + \frac{i}{2}\gamma_{E1}\vec{\sigma}\cdot\vec{E}\times\dot{\vec{E}} - \frac{i}{2}\gamma_{M1}\vec{\sigma}\cdot\vec{B}\times\dot{\vec{B}} - \frac{i}{2}\gamma_{E2}\sigma_i E_{ij}B_j - \frac{i}{2}\gamma_{M2}\sigma_i B_{ij}E_j\right]\psi(x,t). \end{aligned} \tag{1.2}$$

Here

$$\vec{E} = -\frac{\partial\vec{A}}{\partial t} - \vec{\nabla}A_4,\;\; \vec{B} = \vec{\nabla}\times\vec{A},\;\; \dot{\vec{E}} = \frac{\partial\vec{E}}{\partial t},\;\; E_{ij} = \frac{1}{2}(\nabla_i E_j + \nabla_j E_i),\;\; \text{etc.} \tag{1.3}$$

and the various physical quantities are

$$\begin{array}{rl} \mu & \text{magnetic moment} \\ \alpha & \text{electric dipole polarizability} \\ \beta & \text{magnetic dipole polarizability} \\ \gamma_{E1} & \text{electric dipole to electric dipole (E1}\rightarrow\text{E1) spin polarizability} \\ \gamma_{M1} & \text{magnetic dipole to magnetic dipole (M1}\rightarrow\text{M1) spin polarizability} \\ \gamma_{E2} & \text{magnetic dipole to electric quadrupole (M1}\rightarrow\text{E2) spin polarizability} \\ \gamma_{M2} & \text{electric dipole to magnetic quadrupole (E1}\rightarrow\text{M2) spin polarizability} \end{array} \tag{1.4}$$

This effective description of the interaction is expected to be valid for fairly weak fields. The polarizabilities encode rich information on the internal structure of the hadron with varying detail. The same polarizabilities appear in low-energy Compton scattering amplitudes [2], and are actively pursued by experiments and phenomenological studies. Although μ, α and β have been studied in lattice QCD [3], work on spin polarizabilities is just starting [4]. Our goal is to study the feasibility of isolating them on the lattice, combining effective theory and lattice QCD.

2. Lattice discretization

The two-point correlation function in the effective theory (or effective hadron propagator)

$$G_{ss'}(t,\vec{p},A_\mu) = \int d^3x e^{i\vec{p}\cdot\vec{x}} \frac{\int D\psi^\dagger D\psi\, \psi_s(\vec{x},t)\psi^\dagger_{s'}(0,0)e^{-S_{QM}}}{\int D\psi^\dagger D\psi e^{-S_{QM}}}. \tag{2.1}$$

Since the effective action is in the bilinear form $S_{QM} = \psi^\dagger K\psi$, the path integration is easily performed and the resulting correlator $G_{ss'}$ is the inverse of the matrix K. After projection to finite momentum, the correlator is simply a 2 by 2 complex matrix in spin space, with $s = 1,2$ denoting spin up and down.

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We discretize the effective action on a finite lattice of extent $N_xN_yN_zN_t$ and spacing a, and evaluate the inverse numerically using a double-precision BiCGSTAB solver (since K is not hermitian) with a convergence criterion of 10^{-15}. Since the system is non-relativistic, only forward propagation is considered. The derivatives are replaced by appropriate differences on the lattice. We use the unit system in which $\hbar = c = 1$ and $e^2 = 1/137$, and measure all other quantities in terms of fm. So the coordinates (x, y, z, t) are in fm, the nucleon mass $m = 938/197 = 4.76$ fm^{-1}, the nuclear magneton $\mu_N = e/(2m)$ in fm, E and B fields in fm^{-2}, α and β in fm^3, and γ's in fm^4, etc.

Most of the results below are obtained on a $24^3 \times 64$ lattice at $a = 0.1$ fm. The source location is at $(12, 12, 12, 4)$. We use Dirichlet boundary condition in the time direction, and study different boundary conditions in the spatial directions. This is one advantage of the effective approach: we can study boundary conditions exactly as they are in lattice QCD. Another advantage is that we can dial individual terms in the effective action and see their effects in the correlator. No such freedom is afforded in lattice QCD where all relevant terms are present simultaneously. Our basic strategy to determine the polarizabilities is: given a lattice QCD correlator, an effective QM correlator is computed by adjusting the polarizabilities until a match is found.

Below we test the effective QM action with some input values in Table 1 (see [2]). We want to see if the input values could be recovered as output from the effective correlator alone. Such testing is useful because the same methodology can be used on lattice QCD correlators. The advantage here is that the effective QM correlator is fast to compute and free from Monte Carlo noise. Once a method is identified to isolate them, we can determine their true values by matching the effective QM correlator with the corresponding lattice QCD one.

Table 1: Proton and neutron values for testing purposes.

	m (fm^{-1})	μ (μ_N)	α (10^{-4}fm^3)	β (10^{-4}fm^3)	γ_{E1} (10^{-4}fm^4)	γ_{M1} (10^{-4}fm^4)	γ_{E2} (10^{-4}fm^4)	γ_{M2} (10^{-4}fm^4)
p	4.76	2.79	12	2	-3.4	2.7	1.9	0.3
n	4.76	-1.91	12	2	-5.6	3.8	2.9	-0.7

3. Free field

In the case of periodic spatial boundary conditions, which we denote as bc=(1,1,1,0) (the boundary condition in time is always Dirichlet in this study), the correlator projected to zero momentum is a single exponential $G(t) = w\exp(-\lambda t)$ where the spectral weight is $w = 1/(1+am)/a^3$ and the mass of the particle is related to λ by $\lambda = \ln(1+am)$. This was confirmed numerically. In the case of Dirichlet in x and periodic in y and z, denoted as bc=(0,1,1,0), the correlator contains a tower of states with discrete energies

$$G(t) = \sum_{n=1}^{N_x} w_n e^{-\lambda_n t}, \text{ where } \lambda_n = \ln(1+E_n) \text{ and } E_n = m + \frac{p_n^2}{2m}. \tag{3.1}$$

Here p_n is the discrete lattice momentum given by

$$p_n = \frac{\sin(n\pi a/(L_x + a))}{a/2} \text{ with } n = 1, 3, 5, \cdots, \tag{3.2}$$

where L_x is the lattice size in x direction. Note that the even terms are absent under the specific boundary conditions. Since both w_n and λ_n can be calculated exactly in the free-field case, we are able to confirm numerically that the correlator is indeed described by Eq. (3.1) and Eq. (3.2) to double precision. Similar checks were performed for other boundary conditions used in this work: bc=(0,0,1,0), bc=(0,1,0,0), and bc=(1,0,0,0).

4. Constant electric field: α

Next we turn on the electric field. The vector potential $\vec{A} = (-iEt, 0, 0)$ in Euclidean space (we set $A_4 = 0$) corresponds to a real-valued electric field E in the x direction in Minkowski space. We impose Dirichlet boundary condition in the x direction to eliminate the unphysical wrapping-around-the-lattice effects [5] present in lattice QCD so our boundary condition in this case is bc=(0,1,1,0). For neutron, the interaction part of the effective action (all terms except the first two in Eq. (1.2)) is $L_{int} = -1/2\alpha E^2$. We checked that α can be recovered straightforwardly from the correlator for different fields. For proton, the electric field causes an acceleration term in the correlator, in addition to the α term. We checked that α can be cleanly extracted from the unpolarized ratio $G(t,\alpha)/G(t,\alpha=0)$, which not only cancels out the acceleration term, but also the common energy term $m + p^2/(2m)$. The advantage here is that we do not need to know the details of the acceleration: its effects are fully incorporated in the effective QM correlator. Since the acceleration is the same in the effective theory and QCD, its effect can be canceled out in the same way in QCD in the ratio $G_{QCD}(t,\alpha)/G_{QM}(t,\alpha=0)$. This is an alternative method to the one used in previous studies of charged hardons [6].

5. Constant magnetic field: μ and β

Now we turn on the magnetic field. The vector potential $\vec{A} = (0, Bx, 0)$ corresponds to a real-valued magnetic field B in the z direction in Minkowski space. The quantization condition $ea^2B = n(2\pi/N_x)$ would ensure constant B on the periodic lattice, but the fields produced are too strong: the lowest quantized B=306 fm^{-2} on our lattice would cause a proton energy shift of 1.5 GeV from μB (out of 0.938 GeV). One could reduce the strength from another quantization condition $ea^2B = n(2\pi/N_xN_y)$ by 'patching' up the field on the edge of the lattice [7] to ensure uniform flux through every plaquette, but the lowest field (12.8 fm^{-2}) is still too strong for our purposes. So we abandon quantization and use weak fields (as small as B=0.2 fm^{-2}). We impose Dirichlet bc in x and put the source in the center of lattice to minimize the effects from breaking the quantization condition, and Dirichlet bc in y to eliminate the unphysical wrapping-around-the-lattice effects, so bc=(0,0,1,0). For neutron, the interaction in the effective action is $L_{int} = -\mu B\sigma_z - 1/2\beta B^2$. We checked that μ can be recovered from the ratio of polarized correlators $G_{11}(t)/G_{22}(t)$ and β can be recovered from the product $G_{11}(t) * G_{22}(t)$. For proton, there is the additional complication of Landau levels. We checked that the extraction of μ is unaffected since the Landau-level effects cancel out in the ratio. For β, the Landau-level effects can be cleanly removed by taking the double ratio

$$R_\beta = [G_{11}(t,\beta)G_{22}(t,\beta)]/[G_{11}(t,\beta=0)G_{22}(t,\beta=0)]. \tag{5.1}$$

6. Time and space varying fields: γ 's

For γ_{E1}, the choice of the vector potential

$$\vec{A} = (e_1 t^2/a, ie_2 t, 0), \tag{6.1}$$

where e_1 and e_2 are real parameters, gives a time-varying electric field

$$\vec{E} = (-2e_1 t/a, -ie2, 0). \tag{6.2}$$

Because the vector potential has components in both x and y directions, Dirichlet boundary conditions are imposed in these directions to eliminate any wrapping-around-the-lattice effects. The boundary conditions are denoted as bc=(0,0,1,0). The interaction Lagrangian has the form

$$L_{int} = 1/2\alpha(4t^2 e_1^2/a^2 - e_2^2) + \gamma_{E1} e_1 e_2 \sigma_z/a. \tag{6.3}$$

Due to the σ_z dependence γ_{E1} can be isolated from the ratio of polarized correlators

$$R_{\gamma_{E1}} = G_{11}/G_{22} \sim \exp(2\gamma_{E1} e_1 e_2 t/a), \tag{6.4}$$

despite the complicated α term. For proton, the electric field causes an additional acceleration term, but the ratio is not affected and γ_{E1} can be extracted the same way. In both cases (neutron and proton), the method works out nicely numerically. We also checked analytic continuation: $\vec{A} = (e_1 t^2/a, ie_2 t, 0)$ and $\exp(2\gamma_{E1} e_1 e_2 t/a)$ give identical results for γ_{E1} as $\vec{A} = (e_1 t^2/a, e_2 t, 0)$ and $\exp(2i\gamma_{E1} e_1 e_2 t/a)$ for small e_1 and e_2 values.

For γ_{E2}, the choices are

$$\vec{A} = (e_1 y/2, 0, ie_2 tz/a),\ \vec{E} = (0,0,-ize_2/a),\ \vec{B} = (0,0,-e_1/2). \tag{6.5}$$

Dirichlet boundary conditions are imposed in the x and z directions in this case so bc=(0,1,0,0). The interaction Lagrangian has the form

$$L_{int} = 1/2\mu e_1 \sigma_z - 1/2\alpha z^2 e_2^2/a^2 - 1/8\beta e_1^2 + 1/4\gamma_{E2} e_1 e_2 \sigma_z/a. \tag{6.6}$$

The unpolarized α and β terms can be eliminated in the ratio G_{11}/G_{22} which is left with both μ and γ_{E2} terms. Fortunately, the μ term is linear in the fields and γ_{E2} term quadratic. So the μ contribution can be eliminated by averaging the mass shifts over (e_1, e_2) and $(-e_1, -e_2)$. At the correlator level, the eliminations can be achieved simultaneously by the double ratio

$$R_{\gamma_{E2}} = [G_{11}(e_1,e_2)G_{11}(-e_1,-e_2)]/[G_{22}(e_1,e_2)G_{22}(-e_1,-e_2)] \sim \exp(1/2\gamma_{E2} e_1 e_2 t/a). \tag{6.7}$$

The method applies to both charged and uncharged hadrons. It also implies that in order to determine γ_{E2} in QCD we need to perform two lattice QCD calculations: one with an original set of fields, the other with the fields reversed.

For γ_{M2}, the field choices are

$$\vec{A} = (0, e_1 t^2/a, ie_2 t/2),\ \vec{E} = (0,0,-ie_2/2),\ \vec{B} = (-e_1 x/a, 0, e_1 z/a) \tag{6.8}$$

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Dirichlet boundary conditions are imposed in the y and z directions in this case so bc=(1,0,0,0). The interaction Lagrangian

$$L_{int} = \mu e_1(x\sigma_x - z\sigma_z)/a - 1/8\alpha e_2^2 - 1/2\beta e_1^2(x^2+z^2)/a^2 - 1/4\gamma_{M2}e_1e_2\sigma_z/a \tag{6.9}$$

has a similar form as that for γ_{E2}, so the same methodology can be used to extract γ_{M2}. Namely, the double-double ratio in Eq. (6.7) would be proportional to $\exp(-1/2\gamma_{M2}e_1e_2t/a)$.

Finally, for γ_{M1}, no choice of the vector potential can isolate it independently. We found that the choices

$$\vec{A} = (0, ie_1tz/a, e_2x),\ \vec{E} = (0, -ie_1z/a, 0),\ \vec{B} = (-ie_1t/a, -e_2, 0), \tag{6.10}$$

result in an interaction

$$L_{int} = \mu(ie_1t\sigma_x/a + e_2\sigma_y) - 1/2\alpha z^2e_1^2 - 1/2\beta(-e_1^2t^2/a^2 + e_2^2) - 1/4(2\gamma_{M1} - \gamma_{E2})e_1e_2\sigma_z/a, \tag{6.11}$$

that has contributions from both γ_{M1} and γ_{E2}. We can isolate the combination $(2\gamma_{M1} - \gamma_{E2})$ in the same way as γ_{M2}, then use the previously determined γ_{E2} on the same lattice to pin down γ_{M1}. Dirichlet boundary conditions are imposed in the y and z directions in this case so bc=(1,0,0,0).

In summary, these numerical tests demonstrate that all four spin polarizabilities can be disentangled by a judicious choice of the vector potential, and manipulation of effective correlators. The real challenge is whether the same can be done with lattice QCD correlators which are born with Monte Carlo noise.

7. γ_{E1}: a lattice QCD case study

Here we perform a preliminary real lattice QCD simulation to see whether the strategy proposed is feasible. The QCD data are generated on $24^3 \times 48$ lattice with Wilson actions at a=0.093 fm. The field is applied by $\vec{A} = (e_1t^2/a, e_2t, 0)$ and bc=(0,0,1,0), with field values $(e_1, e_2) = (0.23, 0.46)$ fm^{-2}. We analyzed 700 configurations for 6 pion masses from 893 to 404 MeV. In Figure 1, we see that the nucleon ground state starts to dominate at $t = 7$. The effective mass of $\mathrm{Re}[G_{11}(t)]$ is very different in neutron and proton (mostly due to acceleration effects of the proton), but the ratio $\mathrm{Im}[G_{11}(t)/G_{22}(t)] \sim \sin[\gamma_{E1}e_1e_2t/a]$ is the same. The same ratio in QCD suggests a negative γ_{E1} for both neutron and proton, but suffers from large statistical uncertainties. The 3 lines are predictions at 3 different values of γ_{E1} in units of 10^{-4} fm^4. The QCD data suggest a wide range for γ_{E1} (anywhere between 0 and -200). To get a more definitive value for γ_{E1}, the error bars need to be reduced by at least a factor 10, which means the statistics need to be improved by 100 times if no other improvements are made.

8. Conclusion

The effective QM correlator provides a controlled and fast way of examining spin polarizabilities and their systematics on the lattice. By designing the background fields and manipulating the correlators, we have identified methods to isolate all the physical quantities $(\mu, \alpha, \beta, \gamma_{E1}, \gamma_{M1}, \gamma_{E2}, \gamma_{M2})$ for spin-1/2 hadrons as defined in Eq. (1.2). This is possible because of the different field and spin dependences in the terms containing these quantities. By matching with the corresponding lattice

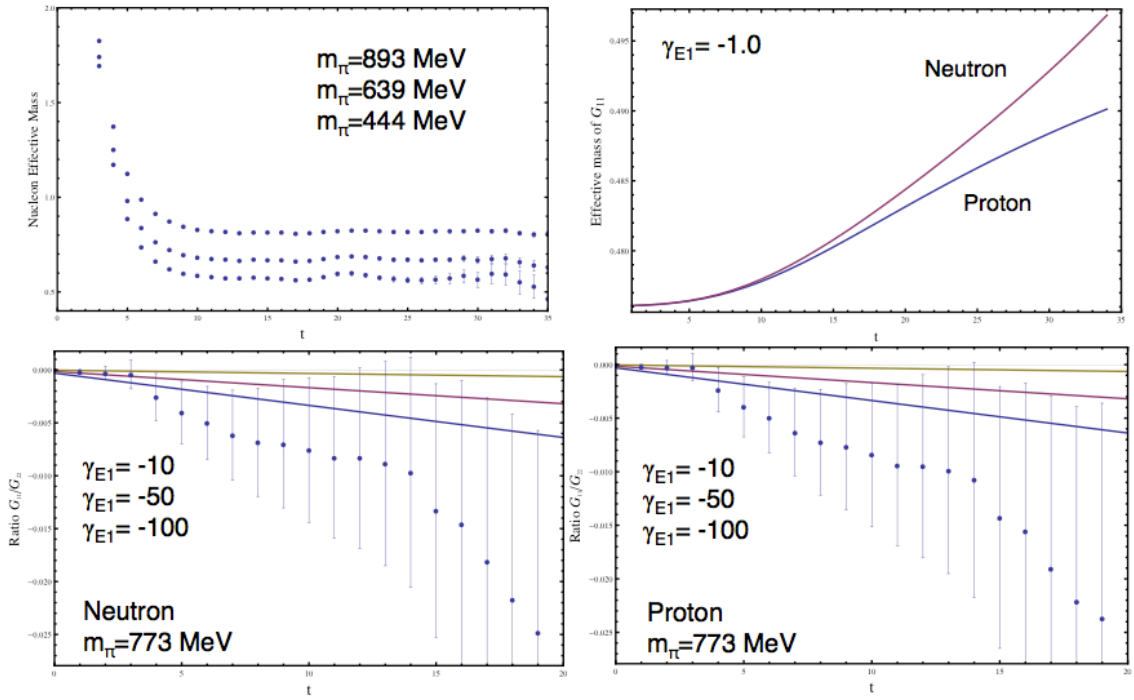

Figure 1: Some results from the γ_{E1} study.

QCD correlators on the same lattice with the same boundary conditions, their QCD values can be determined in principle. A preliminary study of γ_{E1} using lattice QCD data suggests that the challenge lies in the Monte Carlo noise present in the lattice QCD simulations: the noise must be reduced significantly before reliable information can be extracted. Several strategies are being explored to this end.

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