

## Referee Report on: 2112.09336v1

In the manuscript titled “Triplet character of 2D-fermion dimers arising from s-wave attraction via spin-orbit coupling and Zeeman splitting” the authors investigate a fermionic two-component mixture that interacts via short-range interactions, where the particles’ orbital motion is coupled to their spin degree of freedom via spin-orbit coupling. The central finding of this investigation is a two-particle bound state with a triplet character. This result is determined from the observation of the eigenstates from the corresponding Schrödinger equation in combination with Bethe-Peierls boundary conditions. The manuscript is mostly well-written and the results look promising. Therefore, I think that it satisfies the requirement for a publication in SciPost Physics. However, I suggest minor adaptations to increase the comprehensibility of the presented results. In the following part, I elaborate on the main points that should be addressed in the revised manuscript and provide some additional comments for possible improvements.

### Main points

- a. In section 2 the different kinds of spin-orbit coupling are presented in terms of a transformation matrix  $\mathcal{M}$ . I think that already at this stage it should be made clear to the reader that the  $\mathcal{M}$  matrix possesses the property  $\mathcal{M}\mathcal{M}^T = \mathbb{1}$  and hence  $\mathbf{q}^2 = \mathbf{p}^2$  in the case of 2D spin-orbit coupling. In contrast, in the 1D case, the above does not hold and one has  $\mathbf{q}^2 = p_x^2$ . This property elucidates the differences between 1D and 2D spin-orbit coupling and has important ramifications later on, as for instance, it can explain why the different forms of 2D spin-orbit coupling result in the same bound state energy as noted in section 3. Based on the above, I have a few suggestions on how the authors can rectify this issue, which I outline below.
  1. A brief discussion in section 2 should be added about the above-mentioned properties of the  $\mathcal{M}$  matrix.
  2. An explanation, in the beginning of section 3, which addresses that  $\mathcal{M}\mathcal{M}^T = \mathbb{1}$  leads to the bound-state energies being independent of the precise form of the 2D spin-orbit coupling would be useful. In addition, it should be explained that the same is not true regarding the wavefunctions which are sensitive to the form of  $\mathcal{M}$ .
  3. On a related note, in section 5 the authors write “It is possible to transform these results into those applicable to other 2D-type spin-orbit couplings by swapping and/or mirroring the relative-momentum axes according to the structure of  $\mathcal{M}$ -matrices given in Table. 1”. However, no explicit formula is given. Therefore given these issues, the authors should provide an additional appendix where they demonstrate how the wavefunction transforms for the different 2D spin-orbit coupling types.
- b. In Eq. (5) the term  $\mathbf{B}_\mathbf{P} \cdot \boldsymbol{\Sigma}$  is introduced which is then briefly discussed. Considering the results at the end of section 3.2, I think a more to-the-point discussion regarding the properties of this term would be helpful. As a guide to the authors, in the following, I provide a possible interpretation of the results of Fig. 4(b), based on Eq. (5), which they can verify or falsify based on their data and then update the discussion in sections 2 and 3.2 accordingly. First, notice that the above-mentioned term can be rewritten as follows

$$\mathbf{B}_\mathbf{P} \cdot \boldsymbol{\Sigma} = \frac{\lambda \mathbf{Q}^2}{2} (\cos(\theta) \hat{\Sigma}_x + \sin(\theta) \hat{\Sigma}_y) + h \hat{\Sigma}_z \quad (1)$$

where  $\theta$  depends only on the direction of the COM momentum and the specific type of spin-orbit coupling. Therefore, it is obvious that  $\lambda \mathbf{Q}^2$  acts as an effective Rabi-coupling among the spin states and  $h$  is the corresponding Zeeman energy. As a consequence, large amplitudes of the COM momentum favour polarization along the axis  $\mathbf{n} = (\cos \theta, \sin \theta, 0)$  lying on the  $xy$  plane. Large  $h$  give rise to the polarization of the system along the  $z$  spin-axis. The above explains the high  $\mathbf{P}$  results of Fig. 4(b) since for a two-particle system they imply that for large  $\mathbf{Q}^2 = \mathbf{P}^2$  the system is led towards the superposition states  $|1\mathbf{n}_\pm\rangle \equiv e^{I(-\sin \theta \hat{\Sigma}_x + \cos \theta \hat{\Sigma}_y)\pi} |1\pm 1\rangle$  and therefore a population of  $N_{10} \sim 0.5$  and  $N_{1\pm 1} \sim 0.25$  is expected. The deviation of the populations of  $N_{1\pm 1}$  from the above value can be explained by the presence of the term  $\mathbf{q} \cdot (\boldsymbol{\sigma} \otimes \mathbb{1} - \mathbb{1} \otimes \boldsymbol{\sigma})$ , which breaks the SU(2) symmetry associated with  $S$  and couples the states  $|1\pm 1\rangle$  and  $|00\rangle$ .

- c. The derivations in section 2.2 are confusing in my opinion. This particularly applies to those relating to Eq. (23). More specifically, one can easily verify that  $c_\mathbf{P} V_0$  is the normalization

factor of  $|\psi_b\rangle\rangle$  by substituting Eq. (17) and Eq. (21) into  $\langle\langle\psi_b|\psi_b\rangle\rangle$  and noticing that in the case of pure  $s$ -wave interactions the integral over momenta of  $\langle SM|\psi_p(\mathbf{p})\rangle$  vanishes for all cases with  $S \neq 0$ . It is important that the authors comment on this. As it stands, Eq. (23) cannot be used to evaluate  $c_{\mathbf{P}}$  as by substituting Eq. (22) to Eq. (23), the latter reduces to the characteristic equation, Eq. (28). By mentioning that  $c_{\mathbf{P}}V_0$  is the normalization factor of  $|\psi_b\rangle\rangle$  it makes clear why it is independent of  $\mathbf{P}$  and why it does not contribute to Eq. (27) enhancing the readability of this section. The same change also makes clear to the reader that  $|\psi_b(\mathbf{p})\rangle\rangle$  are not orthonormal, a fact which is not mentioned in the current version of the manuscript. In addition, it lifts the ambiguity on how the orbital wavefunctions are calculated in section 5.

- d. For the derivation of Eq. (31) the completeness of the two-body helicity spin-basis,

$$\sum_{\alpha_1, \alpha_2} |\alpha_1, \alpha_2\rangle_{\mathbf{p}, \mathbf{P}} \langle \alpha_1, \alpha_2| = \hat{\mathbf{1}}_{\mathbf{p}, \mathbf{P}}, \quad (2)$$

has to be employed. A property that is not mentioned in the current form of the manuscript. Here  $\hat{\mathbf{1}}_{\mathbf{p}, \mathbf{P}}$  refers to the unity operator within the subspace of fixed relative,  $\mathbf{p}$ , and center-of-mass,  $\mathbf{P}$  momenta. To make the derivation more transparent this property should be added in section 2.1 where the two-body helicity basis is first introduced. This comment should be subsequently referred to in the discussion regarding Eq. (31).

### Minor comments

1. In Eq. (2)  $h$  is introduced but is not defined as denoting the Zeeman energy. The authors should make sure that this quantity is defined in the updated version of their manuscript. In addition, they might consider changing the notation from  $h$  to  $\Delta$  to avoid any possible confusion with the Planck constant.
2. In the discussion following Eq. (3), it might be useful to note that  $\mathcal{M}$  provides a transformation from the configuration to spin space. Moreover, the authors might consider amending the expression regarding  $\hat{\lambda}(\mathbf{p})$  by including the expansion of the matrix multiplications,  $\hat{\lambda}(\mathbf{p}) = \lambda \sum_{a=\{x,y,z\}} \sum_{\mu \in \{x,y\}} \sigma_a M_{a\mu} p_\mu$ . This change will make the distinction between spatial coordinates  $\mu$  and spin coordinates  $a$  clear.
3. Regarding Eq. (10) it should be commented that  $\alpha_1$  and  $\alpha_2$  take values from -1 to 1 and describe the helicity states.
4. In Eq. (23) it might be preferable to denote  $c_{\mathbf{P}}$  as a function  $c(\mathbf{P})$ , or even as  $N(\mathbf{P})$ , where the latter points out its role as the normalization constant.
5. The term ‘‘secular equation’’, might be unfamiliar to some physicists, it might be a good idea to replace it with some more familiar term characteristic or eigenvalue equation.
6. In Eq. (29) the transformation from momentum to real space is only done for the relative coordinate while keeping the COM momentum constant, I think that also the latter fact should be mentioned.
7. During the discussion regarding the reduction to dimensionless quantities, it should be noted that this procedure results in the various quantities mentioned thereafter being measured in the characteristic units of the spin-orbit coupling strength, i.e.  $\hbar = m = \lambda = 1$ .
8. When the dimensionless threshold energy  $\tilde{E}_{\text{th}}$  is introduced in section 3.1, Eq. (15), which defines this quantity, should also be mentioned as a reminder.
9. Additionally, at the beginning of section 3.2 the ‘‘quantity appearing on the r.h.s. of Eq. (37)’’ should be replaced by the concrete specification of the quantity, namely,  $F_{\mathbf{P}}(\epsilon_0, h)$  for  $\mathbf{P} \neq 0$ .
10. The quantity  $\tilde{P}$  is undefined within the main text, with its definition given only in the caption of Fig. 3. The authors should also define it where it first appears in the main text.
11. During the discussion in section 4, it remains unresolved how the  $P_y$  component of the COM affects the results and one has to trace back to Eq. (8) and (9) to verify that it contributes to a  $P_y^2/(2m)$  shift of the bound state energy. The authors should briefly comment on this in section 4.

12. In the end of section 4, to emphasize the fact that “This is important for experiments, as 1D-type spin-orbit coupling is easier to realize, but tuning the interactions to a sufficiently weak strength (e.g. near the zero-crossing of a Feshbach resonance) might prove challenging.”, it would be important to include the appropriate citations.
13. A brief discussion about the envisaged experimental probes should be included in the introduction of the manuscript.
14. In section 6, which describes the possible experimental detection, a criterion referring to a characteristic momentum scale  $m\lambda\sqrt{\tilde{\epsilon}_b + \tilde{\hbar}^2 - 1}$  is derived. The authors should briefly comment on how this momentum scale compares to the resolution that is experimentally achievable considering the typical temperatures in state-of-the-art ultracold atom experiments.