Comment on "Coherent shift of localized bound pairs in the Bose-Hubbard model"

Manuel Valiente,[1,2] David Petrosyan,[1] and Alejandro Saenz[2]
[1]*Institute of Electronic Structure and Laser, FORTH, GR-71110 Heraklion, Crete, Greece*
[2]*Institut für Physik, Humboldt-Universität zu Berlin, D-12489 Berlin, Germany*
(Received 1 December 2009; published 25 June 2010)

We consider scattering of a single particle from an interaction-bound pair of particles in the one-dimensional Bose-Hubbard model. We show that the transmission probability of the single particle is always significantly smaller than unity. This invalidates the main result of L. Jin *et al.* [Phys. Rev. A **79**, 032108 (2009)], where it is claimed that a single-particle wave packet can pass with unit probability through a bound-particle pair and coherently shift its position by one lattice site.

DOI: 10.1103/PhysRevA.81.066101 PACS number(s): 03.67.Lx, 03.65.Ge, 05.30.Jp, 03.65.Nk

In a recent article, Jin *et al.* [1] examined, in the framework of the one-dimensional Bose-Hubbard model, bound states of a pair of particles [2] and scattering of a single particle (SP) from the bound pair (BP). Inasmuch as the complete solution for the bound states of two particles in a lattice had been obtained before [2–4], the main new result of Ref. [1] is that an SP wave packet can pass with unit probability through a BP and shift its position by one lattice site, which could be used to construct a quantum switch that controls coherent transport of the SP. In this Comment, we show that the theoretical model of Ref. [1] is incomplete, and the results are incorrect.

To investigate the scattering between the SP and the BP in the limit of large on-site interaction U (strongly-bound pair), the authors of Ref. [1] employ an effective Hamiltonian, Eq. (16), which reads

$$\tilde{H} = -\kappa \sum_{i=1}^{N} \tilde{a}_i^{\dagger}\tilde{a}_{i+1} + \frac{2\kappa^2}{U}\sum_{i=1}^{N}\tilde{b}_i\tilde{b}_{i+1} - 2\kappa\sum_{i=1}^{N}\tilde{b}_{i+1}^{\dagger}\tilde{b}_i\tilde{a}_i^{\dagger}\tilde{a}_{i+1} + \text{H.c.} + U\sum_{i=1}^{N}\tilde{b}_i^{\dagger}\tilde{b}_i, \quad (1)$$

where $\tilde{a}_i$ and $\tilde{b}_i$ are, respectively, the hard-core bosonic operators for an SP and a BP at lattice site i. The first term describes the SP hopping between neighboring lattice sites with the rate κ, the second term is responsible for the second-order hopping of the BP with the rate $-2\kappa^2/U$, the third term describes the exchange interaction between the SP and the BP at neighboring lattice sites with the rate 2κ, and finally, the last term is the energy U of the BP. By comparing with the effective Hamiltonian H_{eff} derived by us in Ref. [5] to second order in κ, we find, however, that the Hamiltonian of Eq. (1) is missing two more terms,

$$H_{\text{eff}} - \tilde{H} = \frac{4\kappa^2}{U}\sum_{i=1}^{N}\tilde{b}_i^{\dagger}\tilde{b}_i - \frac{7\kappa^2}{2U}\sum_{i=1}^{N}\tilde{b}_i^{\dagger}\tilde{b}_i(\tilde{a}_{i+1}^{\dagger}\tilde{a}_{i+1} + \tilde{a}_{i-1}^{\dagger}\tilde{a}_{i-1}). \quad (2)$$

Here, the first term on the right-hand side is the correction to the internal energy of the BP (or dimer, in the terminology of Ref. [5]), and the second, more important term is the effective nearest-neighbor interaction between the BP and the SP. These terms enter the effective Hamiltonian through the second-order perturbation theory on an equal footing with the BP-hopping term and should, therefore, be retained for consistency. Only in the limit of $|U| \to \infty$ do they disappear together with the BP-hopping term. However, even in this limit, the results on scattering of the SP and the BP obtained in Ref. [1] are incorrect, as we show below. We emphasize that the effective Hamiltonian is valid only in the strong interaction regime $|U|/\kappa > 8$ [5].

By using the effective Hamiltonian H_{eff}, in Ref. [5], we derived the difference relations (7) for the relative coordinate wave function $\phi_K(j_r)$ of the SP and the BP with the total quasimomentum $K = 0, \pm\pi$. There, we obtained the bound solutions of Eqs. (7), while here, we present the scattering solutions. Using the standard ansatz $\phi_k^{(S)}(j_r) = \cos(k|j_r| + \delta_k^{(S)})$ and $\phi_k^{(A)}(j_r) = \text{sgn}(j_r)\cos(k|j_r| + \delta_k^{(A)})$ with k as the relative quasimomentum, for the corresponding phase shifts $\delta_k^{(S)}$ and $\delta_k^{(A)}$ of the symmetric (S) and the antisymmetric (A) scattering wave functions, we readily obtain

$$\tan\left(\delta_k^{(S,A)}\right) = \frac{\bar{J}_K\cos(2k) + (\bar{E} \pm W_K - V^{(2)})\cos(k)}{\bar{J}_K\sin(2k) + (\bar{E} \pm W_K - V^{(2)})\sin(k)}, \quad (3)$$

where $\bar{J}_K = \sqrt{\kappa^2 + J^{(2)2} + 2\kappa J^{(2)}\cos(K)}$, $J^{(2)} = -2\kappa^2/U$, $W_K = 2\kappa\cos(K)$, $\bar{E} = E - (U - 2J^{(2)}) = -2\bar{J}_K\cos(K)$, and $V^{(2)} = -7\kappa^2/(2U)$. Note that in the limit of $|U| \to \infty$, as the nearest-neighbor interaction $V^{(2)}$ and the BP-hopping $J^{(2)}$ tend to zero ($\bar{J}_K \to \kappa$), Eq. (3) holds for all $K = k$. The full scattering wave function is given by a superposition $\phi_k(j_r) = A\phi_k^{(A)}(j_r) + B\phi_k^{(S)}(j_r)$, which, upon being expressed through incident, reflected, and transmitted waves,

$$\phi_k(j_r < 0) = e^{ikj_r} + re^{-ikj_r},$$
$$\phi_k(j_r > 0) = te^{ikj_r},$$

leads to $A/B = -e^{-i(\delta_k^{(S)} - \delta_k^{(A)})}$. For the reflection r and the transmission t amplitudes, we then obtain $r,t = \frac{1}{2}(e^{2i\delta_k^{(S)}} \pm e^{2i\delta_k^{(A)}})$, and the transmission and reflection probabilities are given by $T = |t|^2 = \sin^2(\delta_k^{(S)} - \delta_k^{(A)})$ and $R = |r|^2 = \cos^2(\delta_k^{(S)} - \delta_k^{(A)})$.

In Fig. 1, we plot $T(k)$ for $U/\kappa = -10$ at total quasimomenta $K = 0$ and $|K| = \pi$. The transmission spectra for the intermediate values of K lie in between the curves for $K = 0$ and $K = \pi$. We observe the maximum transmission in the

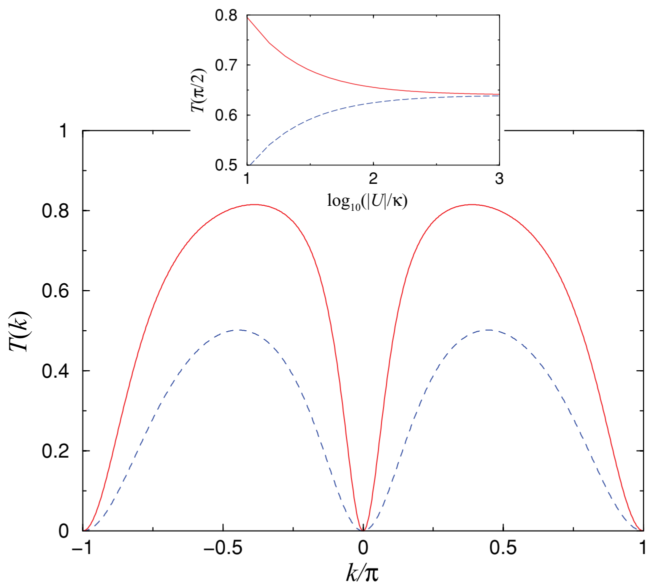

FIG. 1. (Color online) Transmission probability $T(k)$ of a single particle with relative quasimomentum k through a bound-particle pair, for $U/\kappa = -10$ and total quasimomenta $K = 0$ (red solid line) and $|K| = \pi$ (blue dashed line). Inset: single-particle transmission probability at $k = \pi/2$ (corresponding to maximal transmission for $|U| \to \infty$) versus interaction strength $|U|$.

vicinity of $k = \pm\pi/2$, where $T(\pi/2)$ ranges from 50% to 80%. With increasing the interaction strength U, the maximum transmission saturates at around 64% for all values of K, as can be seen in the inset of Fig. 1.

Let us now compare our findings with the corresponding results of Jin *et al.* [1]. These authors claim that for initially separated SP and BP wave packets, each having a certain mean quasimomentum, during the time evolutions governed by Hamiltonian (1), the SP wave packet can pass through the BP with no (or perhaps slight) reflection and shift the position of the BP by one lattice site, which is illustrated in Fig. 2 of Ref. [1]. They do not specify the value of U in their simulation; it appears, however, that they take $|U|$ very large, since the BP wave packet does not disperse or move during the evolution despite having nonzero quasimomentum, it only undergoes a shift of its position by one lattice site due to the exchange interaction with the SP. What we found is that, under no physical conditions, full transmission of the SP through the BP is possible, and significant reflection of the SP wave packet from the BP should always occur for any value of the relative and total quasimomenta and any interaction strength $|U|$, which is large enough for the effective Hamiltonian to be valid. The main reason for this is that the rate of exchange interaction 2κ is twice the rate of the SP-hopping κ, as dictated by the Bose-Hubbard model, precluding perfect transmission of the SP through the BP for any k and K. Stated otherwise, only if the exchange interaction between the SP and the BP were equal to the SP-hopping rate κ, an SP wave packet could completely pass through the BP as if the latter were not there. A less critical point is that, for finite $|U| \gtrsim 10\kappa$, when $T(\pi/2)$ can be relatively large, the nonvanishing nearest-neighbor interaction $V^{(2)}$ induces an effective inhomogeneity of the lattice for the SP, further reducing its transmission through the BP. However, as $|U| \to \infty$, and, hence, $V^{(2)} \to 0$, the maximal transmission probability saturates to a much smaller value of $T(\pi/2) \simeq 0.64$, and the corresponding reflection probability $R(\pi/2) \simeq 0.36$ is much too large to be slight.

Thus, we conclude that the results of Ref. [1] were obtained by replacing in Hamiltonian (1) the correct exchange interaction rate 2κ by κ, which yielded incorrect results. Contrary to the authors' claim, the factor 2 in the exchange interaction, inherent in the bosonic nature of the constituent particles, causes not slight but significant reflection of the SP wave packet from the BP. We have performed time-dependent numerical simulations using both Hamiltonians (1) and (2), and also the full Bose-Hubbard Hamiltonian with three particles, with the initial states used in Ref. [1] and for various values of U/κ, including $|U| \to \infty$. Our simulations confirmed the results of the time-independent scattering calculations based on the correct effective Hamiltonian (2), and we always obtained significant reflection of the SP wave packet from the BP, even when we used the partially incorrect effective Hamiltonian (1) with the correct exchange rate 2κ.

ACKNOWLEDGMENTS

This work was supported by the EU network EMALI.

[1] L. Jin, B. Chen, and Z. Song, Phys. Rev. A **79**, 032108 (2009).

[2] K. Winkler, G. Thalhammer, F. Lang, R. Grimm, J. Hecker Denschlag, A. J. Daley, A. Kantian, H. P. Büchler, and P. Zoller, Nature (London) **441**, 853 (2006).

[3] R. Piil and K. Mølmer, Phys. Rev. A **76**, 023607 (2007); N. Nygaard, R. Piil, and K. Mølmer, *ibid.* **78**, 023617 (2008).

[4] M. Valiente and D. Petrosyan, J. Phys. B **41**, 161002 (2008).

[5] M. Valiente, D. Petrosyan, and A. Saenz, Phys. Rev. A **81**, 011601(R) (2010).