COMMENTS

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Comment on ''Ground-state description of quasi-one-dimensional polarons with arbitrary electron-phonon coupling strength''

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It is shown that the main result presented by Ercelebi and Senger [Phys. Rev. B **53**, 11 008 (1996)] is unreasonable, and is only an artifact produced by a variational scheme rather than an intrinsic property of the system. [S0163-1829(99)01616-1]

In Ref. 1, within a perturbative-variational scheme proposed previously by Devreese *et al.*[2] in the treatment of polarons bound to a Coulomb center, the authors have calculated the binding energy and the effective mass of polarons in a cylindrical quantum wire with infinite potential boundary. The key results obtained in Ref. 1 show that ''at weak coupling, the binding energy of the polaron can be smaller and its mass less inertial compared with the bulk case when the wire is made narrow.'' This is contrary to the general trend that the electron-phonon interaction is inherently stronger in systems of lower dimensionality. We will show that their main results are unreasonable and the general trend is still right.

To show this, we first apply the Feynman-Haken variational path integral method[3] to the Hamiltonian (1) in Ref. 1 and derive the Feynman energy, which is principally an upper bound to true ground-state energy of the system,

$$E^F=\langle\Phi_0^{\rm eff}(\mathbf{r})|[\mathbf{p}^2+V(\rho)]|\Phi_0^{\rm eff}(\mathbf{r})\rangle - \sum_j \sum_{\mathbf{k}} \frac{\langle\Phi_j^{\rm eff}(\mathbf{r})|[v_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}]|\Phi_0^{\rm eff}(\mathbf{r})\rangle|^2}{E_j^{\rm eff}-E_0^{\rm eff}+1}, \qquad (1)$$

where $\Phi_j^{\rm eff}(\mathbf{r})$ and $E_j^{\rm eff}$ are the wave function and ground-state energy of $H_{\rm eff}=\mathbf{p}^2+V_{\rm eff}(\mathbf{r})$. It should be mentioned that $V(\rho)$ is the wire potential taken in Ref. 1 and $V_{\rm eff}(\mathbf{r})$ is the effective potential one should choose in practical calculations. For detailed derivations we refer the readers to Ref. 3, where similar derivations were carried out. It is interesting to note that Eq. (1) will give the results of the second-order Rayleigh-Schrödinger perturbative theory (RSPT) if the effective potential $V_{\rm eff}(\mathbf{r})$ is exactly taken as the confining potential $V(\rho)$. It thus follows that the second-order RSPT provides an upper bound to the exact ground-state energy.

Now, by the second-order RSPT, one can easily obtain the curves of the binding energy E_p (the difference between the ground-state energies of the system in the absence and the presence of the electron-phonon interactions) versus the wire radius R for small α, which is shown in Fig. 1. It is clear that the binding is monotonically stronger as the wire radius R decreases. Because the value of E_p by the second-order RSPT is proportional to α [cf. Eq. (1)], the curves of E_p/α versus R for small α are independent of α and therefore exhibit the same behavior. Because the second-order RSPT provides an upper bound to the exact ground-state energy, Thus, even one obtain the exact results of the ground-state energy of polarons in quantum wire, which may push the E_p-R curves to a higher position, *the values of* E_p *for any wire radius* R *is absolutely not lower than* α, *the value of* E_p *in bulk limit* $R\rightarrow\infty$. Thus, we have strictly shown that the the idea that ''at weak coupling, the binding energy of the polaron can be smaller and its mass less inertial compared with the bulk case when the wire is made narrow''[1] is unreasonable, and the general conclusion that the electron-phonon interaction is inherently stronger in systems of lower dimensionality, which mostly arrived within the second-order perturbation theory, is still qualitatively right.

Next, we will present a few remarks about the results of Fig. 3(a) in Ref. 1 by which the authors arrived at their main conclusions. It is very clear from the curves for $\alpha=0.07$ that almost the whole curve is, surprisingly, considerably less than α, and is therefore more considerably less than the second RSPT ones. As a result of this knowledge, we can con-

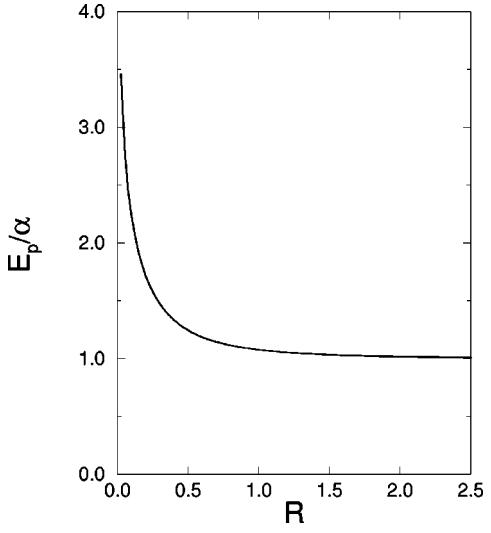

FIG. 1. The binding energy of polarons in quantum wires E_p (in unit of α) within the second-order RSPT as a function of the wire radius R.

vincingly say that the authors obtained very poor results in almost the whole range of the wire radius, not merely in the bulk limit.

In what follows, we will briefly explain why the authors in Ref. 1 obtained such an exceptional property for polarons in quantum wires at weak coupling.

It should be acknowledged that the variational scheme adopted by the author is quite a good approach to deal with a strongly localized state in polaron problems. Here we refer to a state as localized if the root mean square of the coordinate $\mathbf{r}$, calculated by $\{\langle|\mathbf{r}^2|\rangle\}^{1/2}$ with $|\rangle$ being the state, is finite, and extended if it is infinite. For instance, this scheme has been successfully applied to bipolarons,[4] bound polarons,[2] and strong-coupling free polarons[5] and produces very good results in all these problems. These are the expected results due to the fact that a factor $e^{-\lambda^2 r^2}$ or $e^{-\lambda^2 r}$ in the trial states taken in this scheme can only describe the localized states. Note that the operator transformation of Eq. (7) of Ref. 5, which was previously proposed by Huybrechts,[6] is equivalently the introduction of a strong coupling counterpart for a wave function as $e^{-\lambda^2 r^2}$. Of course, the smaller the value of λ is that one finally obtained, the worse is the result obtained by this scheme. In the strong-coupling or strong binding limit, this scheme could present exact results.

For extended states, this scheme will produce very poor results. For example, in Ref. 5 the same authors have shown that this scheme is quite poor in characterizing the free polarons in the weak- and intermediate-coupling regimes. I think this is because the polaron wave function in all directions in the weak- and intermediate-coupling regimes is an extended one. From Fig. 1(a) of Ref. 5, one can clearly see that at the regime $0.03 \leqslant \alpha \leqslant 1$, the binding energy of polarons is lower than that of second-order RSPT theory, and this tendency is more serious with increasing α in the weak- and intermediate-coupling regimes.

For polarons confine in quantum wires at weak coupling, no one can say that the polaron wave function along the wire axis should be a localized one. But in Ref. 1, one can see from the trial state Eq. (17) [substitution of Eqs. (3), (40), and either of Eqs. (39) and (42)] in Ref. 1 that there is a factor $e^{-\beta^2 z^2/2}$ in Eq. (40), which only reasonably describe the localized state along the wire axis. Just by this trial state, which describes the polarons localized along the wire axis, the authors obtained the localized solution at weak coupling for all the wire radius. It is surprising from the curved surface in Fig. 5 of Ref. 1 that at weak coupling and in a wide range of the wire radius ($0 \leqslant R \leqslant 2.0$) the polaron is localized along the wire axis. Note that in the extended state solution, $\xi_z \to \infty$. It is difficult for us to accept that, at such a small coupling constant $\alpha = 0.06$ and for such a large wire radius $R = 2.0$, the longitudinal spatial extent ξ_z is still finite (about 7). This is physically unreasonable. Therefore, in our opinion, at weak coupling this kind of trial state form cannot give physically reasonable results for polarons in quantum wires.

Now we can qualitatively present the cause of these unreasonable properties. The reduction of the wire radius is equivalently the increase of the effective electron-phonon coupling. This statement is true in the literature and also agreed to by the authors in Ref. 1. At weak coupling, when the wires are made narrow, the effective electron-phonon coupling is strengthened and the E_g (ground-state energy) of the polarons in quantum wires becomes decreasing physically. On the other hand, as the effective electron-phonon coupling is enhanced, the results for E_g obtained within this variational scheme become higher than the second-order RSPT results (i.e., E_g is overestimated), which is analogous to the case of free polarons mentioned above and discussed in Ref. 6. According to these combined effects, if the latter effect exceeds the former one, then when the wires are made narrow the polaron ground-state energy would increase, which leads to the decrease of the binding energy E_p. This is exactly the case at $\alpha = 0.07$ in the region of wire radius $0.25 \leqslant R \leqslant 1.0$ in Fig. 3(a) of Ref. 1. As the coupling constant α increases further (it is possible that the former effect always surpasses the latter one for any wire radius), this feature will not show up. So in Ref. 1, when $\alpha > 0.10$, no such feature can be displayed within this variational scheme. In short, at weak coupling the primary reason for this exceptional and incorrect conclusion in Ref. 1 is that the scheme adopted could lead to the overestimation of the ground-state energy of the system.

Finally, we point out that the only ''evidence'' to show that the author's calculation based on Eq. (39) is capable of reflecting a reasonable description of the system over a broader range of R at weak coupling is that Eq. (39) and Eq. (42) in Ref. 1 can give almost identical binding energies for $R \leqslant 2$. In other words, it seems that Eq. (42) could give reasonable results. We disagree. Both Eq. (42) and Eq. (39) are suited in the framework of previous discussions since Eq. (40) is used for both cases. Although the results given by Eq. (42) are better than those given by Eq. (39) at larger R, as shown from by they are still very poor. From the dashed curve, one can easily find that even at $R = 2$ the binding energy given by Eq. (42) is less than α, which in turn is absolutely less than that in the bulk limit. More seriously, these results in Fig. 1 are obviously not self-consistent with their expectation that Eq. (42) depicts asymptotically the bulk limit $R \to \infty$.

Similarly, the above discussion is also suited to the case for the effective mass.

In summary, the main result obtained in Ref. 1 is only an artifact produced by the variational scheme, which is quite poor at weak coupling, rather than an intrinsic property of the polarons confined in quantum wires. It should be pointed out that this method is really a good one for the system at strong coupling.

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