Reply to "Comment on 'Consistent Quantization of Nearly Singular Superconducting Circuits'"

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I. INTRODUCTION

We rebut the principal points made in the Comment. The singular circuit quantization that it introduces is not relevant, as it disagrees with the quantization of the more physical nearly singular circuits. Compactification of circuit variables presents no difficulties. We note some interesting points made in the Comment about the current experimental literature, and we provide some discussion about these. We refer to the paper in question [1] as RD (Rymarz and DiVincenzo) and to the subject Comment [2] as EP-R.

The lossless electric circuits at issue here are pairs of circuits that are related in a particular way: In one (the "nearly singular" one) there are small capacitors present, while in the other ("singular") the small capacitors are rigorously absent. The dynamics, including the quantum dynamics, of the nearly singular circuit are obtained by an uncontroversial analysis, using a Hamiltonian involving the so-called node flux variables [3]. The related singular circuit cannot be quantized by this route, the reason being that its Lagrangian (which is straightforward to write down) cannot be Legendre transformed to a Hamiltonian, due to the noninvertibility of the capacitance matrix.

For the purpose of this Reply, we focus entirely on the particular circuits shown in EP-R as Figs. 1(b) (nearly singular) and 1(c) (singular).

The formal question of how to quantize the singular circuit has arisen. The problem is not a new one, and an analysis procedure can be adopted. RD refers to this procedure as Dirac-Bergmann (DB), after two of the famous authors who have developed such prescriptions, although the names Faddeev and Jackiw can also be mentioned. But, for the singular electric circuit, the DB analysis procedure boils down to a simple prescription: Use the Kirchhoff current law to eliminate node-flux variables in the Lagrangian before Legendre transforming. For the simple singular circuit shown as Fig. 1(c) of EP-R, there is a parameter range $\beta < 1$ [cf. Eq. (1) of EP-R] where this application of the Kirchhoff current law gives a Hamiltonian function which can be quantized, so it constitutes an internally consistent mathematical procedure—but one that does not give the correct quantum dynamics of the nearly singular circuit.

Looking more closely at this DB-generated Hamiltonian, it is derived as follows (see EP-R Fig. 1): One eliminates the variable ϕ_c (which has no kinetic energy due to $C_J = 0$) in the classical Lagrangian, leaving a Lagrangian for the single remaining variable ϕ. After this, via a Legendre transform, one obtains the classical Hamiltonian which includes a potential $U_{\mathrm{DB}}(\phi)$. One then quantizes this system. For $\beta < 1$, $U_{\mathrm{DB}}(\phi)$ is single valued; for $\beta > 1$, $U_{\mathrm{DB}}(\phi)$ is multivalued, making it clear that one cannot proceed further with DB.

Let us summarize the alternative provided by our work (RD): We start by keeping both variables in the classical Lagrangian with C_J finite. We derive the classical Hamiltonian and then quantize the system. Only after quantization at finite C_J do we consider the singular limit $C_J \to 0$. For small C_J, we show that one can eliminate the additional fast degree of freedom ϕ_c using a Born-Oppenheimer (BO) approximation, which puts this degree of freedom into its quantum ground state. Indeed, the BO approximation is increasingly accurate as C_J approaches 0.

We show that $U_{\mathrm{BO}}(\phi) \neq U_{\mathrm{DB}}(\phi)$—the effective potential $U_{\mathrm{BO}}(\phi)$ for the remaining degree of freedom is entirely different from the one obtained by the DB procedure—including in the limit $C_J \to 0$. At an intuitive level, the

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reason for this discrepancy is that, quantum mechanically, there is the zero-point energy, and associated zero-point fluctuations, of the eliminated degree of freedom ϕ_c, while in DB ϕ_c is taken to have a fixed function of ϕ without any additional fluctuations.

This difference between $U_{\mathrm{BO}}(\phi)$ and $U_{\mathrm{DB}}(\phi)$ was already shown to be significant in our previous work [4] for moderate values of C_J; see Fig. 2.12(a) for $\beta = 0.7$. In RD, we prove (Theorem 1) that, in the limit $C_J \to 0$, $U_{\mathrm{BO}}(\phi)$ becomes a zero-point constant, *independent* of ϕ. We prove that this is a fixed-point flow behavior and that this fixed point is shared by a large family of other circuits [e.g., Fig. 1(a) of EP-R].

II. ITEMIZED REPLY

To address EP-R's criticisms more directly, we provide here a discussion of their points, organized according to the "three arguments" in EP-R, starting on p. 2.

Argument I: Classical adiabatic limit.—In RD Sec. II B, the cosine potential has been chosen to provide an example featuring the well-known nonlinearity of the Josephson junction. In principle, any other sufficiently well-behaved, subparabolic potential would similarly suffice for the subsequent analysis, leading to RD's Theorem 1. In RD, we show that the effective Hamiltonians in Eqs. (12) and (18), and consequently their spectra, generally do not coincide. This discrepancy between the results obtained through the classical adiabatic approximation followed by quantization (i.e., the procedure of EP-R), and those derived from quantization followed by a quantum adiabatic approximation, represents the type of failure RD identifies. To be explicit, we find that Eq. (14) of EP-R is an incorrect effective potential, particularly for the circuit in Fig. 1(b) for small C_J.

For the cosine potential, we agree that the classical adiabatic approximation breaks down for $\beta > 1$. But this breakdown is not the problem or the type of "failure" with DB that is identified in RD. The failure is the inequality of the effective Hamiltonians (classical adiabatic elimination vs quantum adiabatic elimination), and it arises for all values of β (although the problem is less in the vicinity of $\beta = 0$; see the discussion of Argument III below). This and other items of relevance in this Reply were extensively studied in the Master's thesis of Rymarz [4].

In the course of their argument, EP-R impugn the BO approximation, without providing details. Although not emphasized in RD, Theorem 1, in employing the BO procedure, provides a means of obtaining the full spectrum up to high energy—actually, up to an energy scale set by the fast-variable zero-point energy scale, which diverges as $C_J \to 0$. As pointed out by EP-R, RD does *not* give any rigorous proofs of the applicability of the BO approximation. We invoke physical experience here and the various computations reported already in Ref. [4]. Again, a well-known feature of BO is that, if the fast-slow ratio is big enough, the range of energies within which the spectrum is reliable is quite large. (The traditional BO approximation of molecular physics can accurately predict the entire infrared rotovibrational spectrum of many important molecules, and the zero-point scale at which the BO approximation has to be modified is often in the ultraviolet.)

We do not plan to work on a program of making the BO approximation mathematically rigorous; in looking at what has been done, starting in the 1970s, it would clearly take another deep dive into the work of Reed and Simon [5]. But we rest on the 50 years of experience in using the BO approximation as a physical theory, before there were any rigorous proofs of its validity. We would finally observe that the problem that we are discussing in this case [Fig. 1(b) of the Comment of EP-R] is easy enough that, with care, it can be reliably solved numerically—it just requires the solution of a 2D Schrödinger equation, which can be accurately discretized and solved on a computer. The evidence from Ref. [4] is that solving directly reveals that the wave function ansatz of the BO approximation is already well satisfied for moderately small C_J and that the tendency of the eigenspectrum to approach that of the free rotor (or free particle, in the noncompact point of view) is already quite evident in such numerics.

Here and in the Supplement part of the Comment, EP-R, when accepting the validity of BO, seem to imply that two models (DB and BO) agree just because they both have a purely continuous spectrum (taking the noncompact point of view). This is by no means the case. It is not correct to call two spectra the same if they are both continuous spectra (sometimes called scattering spectra). For the two models being discussed here, the two spectra disagree in their energy onset, in their density of states (which, among other things, determines the so-called band-edge masses), and in the position and size of band gaps. In the correct spectrum, these gaps in the continuous spectrum are all vanishing as $C_J/C \to 0$, while for the Hamiltonian of EP-R [their Eq. (5)] the gaps are all finite for their circuit in Fig. 1(c) (Josephson junction case). To see an excellent account of how such band gaps depend on the form of a 1D periodic potential, it is instructive to consult the original Kronig and Penney 1931 paper [6].

Argument II: Compact or noncompact?—EP-R state that they detect an implicit assumption in Sec. III of RD that the variable ϕ_c is noncompact. In fact, RD on purpose refrained from indicating any such assumption, because it is clear that the results there apply whether or not ϕ_c is considered to be compact or extended. This point has already been explicitly stated as Ref. [45] of RD. It was our intention from the beginning to make the results here usable, no matter which "camp" one happens to belong to. This easy transition from extended to compact rests on a few observations: (i) A simple observation that RD neglected to make (but was clear in Ref. [4]) is that if U_{NL} is periodic, and, thus, can be potentially viewed as compact, then U_{BO}

is also periodic for any nonzero value of C_J (or of κ in the EP-R notation). In this case then, U_{BO} for the effective reduced system can also be viewed as compact. (ii) If U_{NL} is periodic, then the eigenspectrum of the problem, in the noncompact view, obeys Bloch's theorem. This is just a statement that the eigenfunctions must belong to irreducible representations of the translation group. Then, the discrete eigenspectrum of the compact version of the model is obtained by simply selecting the states from one of the irreducible representations (that with $k = 0$, in the band-structure language, if there is no offset charge). We point out that the BO ansatz also respects Bloch's theorem.

Thus, we cannot accept the view of EP-R that the BO approximation can be good for the noncompact problem but bad for the compact version of the problem. Among the continuous spectrum of states that are obtained in solving the Hamiltonian derived with the BO approximation (noncompact), the point-spectrum solutions of the compact version of the problem have, thus, already been obtained—no further or alternative approximations need to be made.

Given the intimate relation between the compact and noncompact spectra, we can explain why we consider all compact problems as belonging to our type 1 definition of nonlinear inductors. The reasoning is just to "decompactify" the domain, thus associating the compact U_{NL} with the corresponding periodic function on the noncompact space. Then, the classification criteria can be applied and put any such potential in the type 1 category (a or b). Finally, any conclusions about the eigensolutions of the problem can be transferred back to the compact problem by the "$k = 0$ selection" stated above.

In the Appendix, we comment on fallacies in EP-R's analysis of the quantum adiabatic limit for supposedly compact variables in the Josephson junction case.

Argument III: [Alleged] lack of experimental evidence.—EP-R bring forward a set of experimental results, old and new, which they feel are not aligned with RD. The examples of EP-R are diverse and interesting; several of them are not so much experiments as issues raised in the modeling of experiments. None of them are, in fact, in contradiction with RD, but they raise a variety of important issues that are worth commenting upon.

In many examples, singular circuits are invoked to explain some aspect of experiment—that is, circuits for which the capacitance matrix is not invertible. Of these, many involve a chain of Josephson junctions [7,8]; there are, in fact, many other examples in the literature. These works give the impression that one obtains an effective inductive response by series addition (invoking Kirchhoff's current law) of nonlinear inductances. RD would argue that, in the limit of very small capacitances, quantum fluctuations would erase the inductive response ($U_{\mathrm{BO}} \to 0$).

This is clearly not the case experimentally. But neither are the capacitances (shunting or to ground) actually infinitesimal. It is implicitly understood that they are in a "not very small" range, so that, in fact, the quantum fluctuations of the phases along the chain are fairly small. Thus, the classical reasoning is not so far off. Within the experimental community there is an understanding (but unfortunately not entirely widespread) that the junction capacitance should for this reason not be extremely small and that one, in fact, strives for a kind of "transmon regime"; see also RD Sec. IV A 1. There have been papers (e.g., Yale group analysis of SNAIL elements; see the analysis of Fig. 1 in Ref. [9]) in which the relatively small fluctuation suppression of the effective Josephson energy has been carefully calculated. On the other hand, the recent work in Ref. [7] misses the importance of small capacitances and misquotes the conclusion of RD on this point.

Thus, RD is not in contradiction with any of this but provides a warning that chain capacitances, if too small, would suppress the desired "superinductance" effect.

In other examples [10] provided by EP-R, the singular effect (absence of nodes with capacitances) occurs in a linear part of the circuit. As stated in RD, linear cases like this are harmless—taking these capacitances to zero, while leading to diverging quantum fluctuations, still leads to agreement with normal series-combination laws.

In the transmon example discussed by EP-R, and in Ref. [11], it is noted by EP-R that it seems that it can be assumed that one does normal series-combination arguments, neglecting extra capacitances. We agree that we should have made some note of this in Ref. [11] (DiVincenzo is an author of that work). It should be noted that the cases at issue are exactly the canonical circuit of RD, but with $\beta \ll 1$. There is, in fact, an interesting interplay of small L and small C_J, such that, if L is sufficiently small, there is a significant range of small but finite C_J in which the series-combination rule is quite accurate, even though it ultimately fails when C_J is taken even smaller. The work in Ref. [11] implicitly assumed that C_J was falling in this range and so could be neglected.

Thus, we agree that analyses involving series-combination rules (DB, if you will) are sometimes satisfactory. But we disagree on what the regimes of applicability are: For our circuit, EP-R say that the failure occurs at $\beta = 1$ (which they also refer to as a "singular point"), while we say that the applicability is restricted to $\beta \ll 1$.

Finally, EP-R points out the fundamental early work of Golubov, Kupriyanov, and Il'ichev [12] and Il'ichev *et al.* [13] on physical models of two-terminal devices leading to a variety of Josephson-like characteristics (alternative periodic phase-current relations). Among these are characteristics that exactly match the L-JJ series combination that RD has criticized. We would reply that such device models are naturally understood to have a specific range of validity (frequency ranges, for example), which would imply the presence of other parasitics in a more exact model. Furthermore, the devices of earlier decades were often rather "classical" (large parameter values), so that

quantum-fluctuation effects can be neglected. It is well known that, in such a classical limit, various interesting phenomena occur for $\beta > 1$, in particular, multistability. But these phenomena must be reconsidered in the "modern" setting in which quantum fluctuations can play a very significant role.

III. FINAL REMARKS

We can close by reflecting on some aspects of the solution to the classical dynamics of their Fig. 1(b) that EP-R may have overlooked. It is true that the classical dynamics has a 1D slow manifold, whose embedding in the 2D coordinate space is given by Kepler's equation, EP-R's Eq. (2). In the adiabatic limit, if the system is started at rest on this manifold, it will travel slowly along this manifold. But one should not proceed to quantize this 1D motion, because, if the initial condition does not lie on this manifold, the classical motion is quite different: The system will experience fast oscillatory (transverse) motion around the 1D manifold, while additionally drifting slowly along it.

These fast and slow motions are coupled because of the anharmonicity, so that the parametric slow motion is a function of the amplitude of the rapid transverse oscillation. Classical physics does not constrain the amplitude of this transverse motion (although see the aside in the next paragraph); but quantum mechanics does constrain it. In the quantum setting, this motion cannot have zero amplitude; its size is set by Bohr-Sommerfeld quantization, so that there is a certain minimal transverse motion, which is the "zero-point fluctuation." In the extreme quantum case, $C_J \to 0$, this transverse motion significantly renormalizes the parametric slow motion. This is a classical explanation of the $U_{\mathrm{BO}} \to 0$ tendency that RD has identified.

A final aside: The EP-R 1D manifold assumes higher importance in the classical dynamics if there is a moderate amount of viscosity. In this case, the fast transverse motion can be strongly overdamped, but the slow motion very underdamped, so that in this case trajectories will indeed spend most of their time on the slow manifold determined by the Kepler equation (at least for $\beta < 1$). But this viscous theory is not the one that we quantize.

APPENDIX: BORN-OPPENHEIMER APPROXIMATION FOR PERIODIC U_{NL}

We emphasize that, in contrast to the claims made by EP-R in their Argument II and their Supplemental Sec. IV, neither an intrinsic scale nor a "compact" ϕ_c affect the application of the BO approximation. First of all, note that nonperiodic potentials defined on $\mathbb{R}$ can also provide a natural flux scale (e.g., the fluxonium potential), which, however, does not "skew" the hierarchy fast and slow as claimed by EP-R. Although EP-R correctly observe that their Hamiltonians in Eqs. (7) and (15) are related by a dilation transformation, they consider different fast Hamiltonians for both representations of H_r; but the (rescaled) choice of H_{fast} in Eq. (8) is an equally adequate fast Hamiltonian for both H_r in Eq. (7) and H_r in Eq. (15), naturally resulting in equivalent descriptions of the system featuring identical spectra. However, EP-R consider the choice $H_{\mathrm{fast}} \propto n_c^2$ for H_r in Eq. (15), which does not correspond to the "electronic Hamiltonian" of the system [i.e., the sum of the "small-mass" kinetic terms and the potential terms; see RD Eq. (16) and Ref. [68]] as would be the case for a conventional BO approximation. EP-R's choice of H_{fast} does not depend on φ_c at all. Consequently, they misleadingly identify a breakdown of the adiabatic separation for the extended case and thereby a seeming dissimilarity between the "extended" and "compact" cases. In the following, we comment on the quantum mechanical description of the system.

For the extended case, EP-R correctly point out that the spectrum of n_c would be the entire real line, and they conclude that $H_{\mathrm{fast}} \propto n_c^2$ does not represent a proper fast Hamiltonian for a BO approximation. In their words, "the determination of the slow Hamiltonian is not achieved simply through reading out the coefficients of various terms of the full Hamiltonian." This conclusion, however, should initiate a reconsideration of H_{fast} (also for the compact case) as no particular assumption on U_{NL} has been made (apart from an intrinsic scale), and two-dimensional systems with extended variables are considered by EP-R the "harmless" case for the application of a BO approximation.

For the supposedly "compact" case, however, EP-R restrict the flux variable to the circle and insist on an integer spectrum of n_c, although for a fixed value of φ, the Hamiltonian in EP-R Eq. (15) is not periodic in φ_c, even with a periodic extension of U_{NL} in order to "decompactify" its domain; see the discussion of Argument II in the main text above. In other words, the system cannot be in the same state before and after a full orbit of φ_c on the circle for a fixed value of φ, or the (absolute) values of the wave function do not coincide at the domain borders of φ_c for a fixed value of φ (as required for a circle). Thus, n_c does not have to be an integer multiple of $2e$, as the electric charge can continuously flow through the linear inductor. Regardless of these implausible restrictions to the integer spectrum of n_c and the circle domain of φ_c, EP-R's choice of the fast Hamiltonian leads to further problems in their analysis made in Supplemental Sec. V B. There, EP-R naturally conclude that the spectrum of their fast Hamiltonian is independent of φ, and they derive their effective Hamiltonian in the form of a shifted harmonic oscillator by computing the (operator-valued) expectation value of the slow Hamiltonian in the ground state of their fast Hamiltonian, which has a wave function that is constant on its domain. Note that such an expectation value depends on the domain of φ_c; e.g., it differs for the choices $\varphi_c \in [0, 2\pi)$ and $\varphi_c \in [-\pi, \pi)$, which is nonsensical if φ_c lives on a circle. This dependency on the domain is not mentioned by EP-R, as a shift of the harmonic oscillator

does not affect its spectrum. However, it will crucially change the spectrum as soon as H_r is not quadratic in $\varphi - \varphi_c$, which is the case if the linear inductor is replaced by a nonlinear one. Finally, the problematic choice of the fast Hamiltonian is also demonstrated by the fact that—taking the overall energy scale E'_C in EP-R Supplemental Eq. (20) into account—the spectrum of EP-R's effective Hamiltonian (i.e., the properly scaled shifted harmonic oscillator) depends neither on U_{NL} nor C' at all, although the limit $\kappa \to 0$ has not been considered (yet).

To complete the discussion of the BO approach for periodic U_{NL}, we comment on the dilation transformation discussed by EP-R: Note that the identification of the fast Hamiltonian and the spectrum of both the fast Hamiltonian as well as of the final effective Hamiltonian and the validity of the BO approximation do not depend on such a dilation transformation, even if the rescaling of a variable is singular as $\kappa \to 0$. However, in their Supplemental Sec. IV D, EP-R claim that the equivalence between the Hamiltonians in their Supplemental Eqs. (5) and (20) is suspect in the limit $\kappa \to 0$. Such an equivalence of the Hamiltonians in the limit $\kappa \to 0$ prior to applying the BO approximation has not been considered and is not required in RD, because a rescaling of the fast variables does not affect the BO potential. Moreover, in RD, only the one-dimensional "electronic" subproblem, i.e., the fast variables (with extended domains due to the quadratic term in the correctly identified fast Hamiltonian), have been rescaled, and the potential issues with a two-dimensional dilation transformation are an artifact introduced by the allegedly controversial adimensionalization of EP-R. Their concerns might originate from the fact that, although EP-R state that "dilations are not canonical transformations of the cylinder" and that a dilation "maps from one cylinder to another, different, cylinder, changing its radius," they apparently insist on unchanged symmetries of the Hamiltonian; cf. their Supplemental Sec. IV F. However, it should be clear that the boundary conditions of the underlying Schrödinger equation (i.e., the periodicity or the interval or domain of the wave functions) are naturally changed by a dilation transformation. Consider the following simple example: On the one hand, the eigenfunctions $\psi(\varphi)$ of the standard CPB or transmon Hamiltonian $H_{\mathrm{CPB}} = 4E_C(n - n_g)^2 - E_J\cos(\varphi)$ with $[\varphi, n] = i$ satisfy $\psi(\varphi + 2\pi) = \psi(\varphi)$. Here, the Cooper pair number operator n has an integer spectrum. On the other hand, the CPB Hamiltonian is related to $\tilde{H} = 4E_C(\tilde{n}/2 - n_g)^2 - E_J\cos(2\tilde{\varphi})$ with $[\tilde{\varphi}, \tilde{n}] = i$ via a dilation transformation. Obviously, the eigenfunctions of $\tilde{H}$ satisfy $\tilde{\psi}(\tilde{\varphi} + \pi) = \tilde{\psi}(\tilde{\varphi})$, and the spectrum of the electron number operator $\tilde{n}$ is restricted to all even integers $0, \pm 2, \pm 4, \ldots$, which is not equivalent to that of n. These observations have to be compared with the claims in EP-R's Supplemental Sec. IV F, stating that "a transformation […] would change the spectrum, and spectra are invariant under unitary conjugation".

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