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Title	Emergent thermodynamics in a quenched quantum many-body system
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Publication date	2012
Original Citation	Dorner, R., Goold, J., Cormick, C., Paternostro, M. and Vedral, V. (2012) 'Emergent thermodynamics in a quenched quantum many-body system', Physical Review Letters, 109(16), 160601 (5pp). doi: 10.1103/PhysRevLett.109.160601
Type of publication	Article (peer-reviewed)
Link to publisher's version	https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.109.160601 - 10.1103/PhysRevLett.109.160601
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Download date	2026-11-06 05:04:11
Item downloaded from	https://hdl.handle.net/10468/4622



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Emergent Thermodynamics in a Quenched Quantum Many-Body System

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(Received 27 July 2012; published 18 October 2012)

We study the statistics of the work done, fluctuation relations, and irreversible entropy production in a quantum many-body system subject to the sudden quench of a control parameter. By treating the quench as a thermodynamic transformation we show that the emergence of irreversibility in the nonequilibrium dynamics of closed many-body quantum systems can be accurately characterized. We demonstrate our ideas by considering a transverse quantum Ising model that is taken out of equilibrium by an instantaneous change of the transverse field.

DOI: 10.1103/PhysRevLett.109.160601 PACS numbers: 05.70.Ln, 05.30.Rt, 05.40.−a, 64.60.Ht

Introduction.—In the past decade or so, there has been a revival of interest in the study of nonequilibrium dynamics in closed quantum systems. Mainly, this is due to a series of spectacular experiments using ultracold atoms, where the high degree of isolation and long coherence times permit the study of dynamics over long time scales [1]. These experiments have raised a number of important theoretical issues including the relationship between thermalization and integrability [2] and the universality of defect generation in the crossing of a critical point [3]. A common way to take a many-body system out of equilibrium is by an abrupt change of a local or global parameter of the Hamiltonian, this is commonly referred to as a "sudden quench." Following a quench the dynamical response of the system can be probed by studying, for example, the dynamical correlation functions [4], the change in the diagonal entropy [5] or the statistics of the work done [6].

Over a similar period of time, there has also been a great deal of interest in the statistical mechanics community surrounding the discovery of the nonequilibrium fluctuation relations (see, e.g., Ref. [7] for a review). Essentially, the fluctuation relations encode the full nonlinear response of a system to a time-dependent change of a Hamiltonian parameter. In particular, they make a definitive statement regarding the irreversible entropy production in a system following a thermodynamic transformation and, as such, allow us to understand the emergence of thermodynamic behavior in systems where the microscopic laws are inherently reversible. Given the current experimental interest in the nonequilibrium dynamics of ultracold atomic systems and the recent developments in statistical mechanics, it is natural to study the quench dynamics of quantum many-body systems in this new thermodynamical formulation. In this work we use the transverse quantum Ising model [8] to provide an exact analysis of the Tasaki-Crooks and Jarzynski fluctuation relations in a quenched many-body system. Furthermore, we compute the irreversible entropy production and show that the emergence of thermodynamics provides an elegant interpretation of the essential physics.

Nonequilibrium quantum thermodynamics.—We begin by reviewing some key concepts of microscopic thermodynamics, allowing us to define the formalism that is used in the rest of our study.

One of the fundamental goals of quantum thermodynamics is to understand how thermodynamical laws emerge from the underlying quantum mechanics of individual particles [9]. In this spirit, we consider a dynamical system described by a Hamiltonian $H(\lambda(t))$ that depends on an external work parameter $\lambda(t)$, i.e., an externally controlled parameter whose value determines the equilibrium configuration of the system. The system is prepared by allowing it to equilibrate with a heat reservoir at inverse temperature β for a fixed value of the work parameter $\lambda(t \leq 0) = \lambda_0$. The initial state of the system is thus the Gibbs state $\rho_{\mathrm{G}}(\lambda_0)$, where

$$\rho_{\mathrm{G}}(\lambda) := \frac{e^{-\beta H(\lambda)}}{\mathcal{Z}(\lambda)},$$

and the partition function is $\mathcal{Z}(\lambda) := \mathrm{Tr}[e^{-\beta H(\lambda)}]$. At $t = 0$ the system-reservoir coupling is removed and a protocol is performed on the system taking the work parameter from its initial value λ_0 to a final value λ_τ at a later time $t = \tau$. The initial and final Hamiltonians connected by the protocol $\lambda_0 \rightarrow \lambda_\tau$ have the spectral decompositions $H(\lambda_0) = \sum_n \epsilon_n(\lambda_0)|n\rangle\langle n|$ and $H(\lambda_\tau) = \sum_m \epsilon'_m(\lambda_\tau)|m\rangle\langle m|$, respectively, where $|n\rangle$ ($|m\rangle$) is the nth (mth) eigenstate of the initial (final) Hamiltonian with eigenvalue ϵ_n (ϵ'_m).

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The definition of the work done on the system W as a consequence of the protocol requires two projective measurements: The first projects onto the eigenbasis of the initial Hamiltonian $H(\lambda_0)$ at $t = 0$, with the system in thermal equilibrium. The system then evolves under the unitary dynamics $U(\tau; 0)$ generated by the protocol $\lambda_0 \rightarrow \lambda_\tau$ before the second measurement projects onto the eigenbasis of the final Hamiltonian $H(\lambda_\tau)$. The probability of obtaining ϵ_n for the first measurement outcome followed by ϵ'_m for the second measurement is then $p^0_n p^\tau_{m|n} = e^{-\beta\epsilon_n}|\langle n|U(\tau, 0)|m\rangle|^2/\mathcal{Z}(\lambda_0)$. Accordingly, the work distribution is defined as [10]

$$P_{\mathrm{F}}(W) = \sum_{n,m} p^0_n p^\tau_{m|n} \delta(W - (\epsilon'_m - \epsilon_n)). \tag{1}$$

Equation (1) therefore encodes the fluctuations in the work that arise from thermal statistics (p^0_n) and from quantum measurement statistics ($p^\tau_{m|n}$) over many identical realizations of the protocol. For our purposes, it is convenient to define the characteristic function of the work distribution as the Fourier transform of Eq. (1) [11]

$$\begin{aligned}\chi_{\mathrm{F}}(u, \tau) &:= \int dW e^{iuW} P_{\mathrm{F}}(W) \\ &= \mathrm{Tr}[U^\dagger(\tau, 0) e^{iuH(\lambda_\tau)} U(\tau, 0) e^{-iuH(\lambda_0)} \rho_{\mathrm{G}}(\lambda_0)].\end{aligned} \tag{2}$$

The convenience of $\chi_{\mathrm{F}}(u, \tau)$ is evident when considering the well-known Tasaki-Crooks fluctuation relation $P_{\mathrm{F}}(W)/P_{\mathrm{B}}(-W) = e^{\beta(W-\Delta F)}$ [10,12]. This states that the ratio between the *forward* work distribution $P_{\mathrm{F}}(W)$, introduced above, and the *backward* work distribution $P_{\mathrm{B}}(-W)$, obtained from the protocol $\lambda_\tau \rightarrow \lambda_0$ in which the system is initialized at $t = 0$ in the Gibbs state $\rho_{\mathrm{G}}(\lambda_\tau)$ and evolves according to $U^\dagger(\tau, 0)$, is related to the difference in the equilibrium free-energy of the system ΔF. Following Ref. [13] the Tasaki-Crooks relation is written in terms of the characteristic function as

$$\frac{\chi_{\mathrm{F}}(u, \tau)}{\chi_{\mathrm{B}}(-u + i\beta, \tau)} = \frac{\mathcal{Z}(\lambda_\tau)}{\mathcal{Z}(\lambda_0)}, \tag{3}$$

where we have introduced the backward characteristic function $\chi_{\mathrm{B}}(v) := \int dW e^{ivW} P_{\mathrm{B}}(W)$, with the complex argument $v = -u + i\beta$. Moreover, the Jarzynski equality [14] is easily obtained from Eq. (2) by introducing the parameter $u = i\beta$, giving

$$\chi_{\mathrm{F}}(i\beta, \tau) = \langle e^{-\beta W}\rangle = \frac{\mathcal{Z}(\lambda_\tau)}{\mathcal{Z}(\lambda_0)} = e^{-\beta\Delta F}, \tag{4}$$

where in obtaining the last equality we have used the relation $\Delta F = -(1/\beta)\ln[\mathcal{Z}(\lambda_\tau)/\mathcal{Z}(\lambda_0)]$. Both the Tasaki-Crooks and Jarzynski fluctuation relations are statements regarding the symmetry of fluctuations in work during thermodynamic transformations of microscopic systems. Remarkably, these symmetries are solely determined by the equilibrium state quantity ΔF regardless of how far the system is driven from equilibrium. For a recent information-theoretic interpretation of the fluctuation relations see Ref. [15].

Irreversible entropy production.—For finite systems, the statistical nature of work Eq. (1) requires the second law of thermodynamics to be revised to the form $\langle W\rangle \geq \Delta F$, with equality being reached for a quasistatic process. For all nonideal processes, the deficit between the average work $\langle W\rangle$ and the variation in free energy can be accounted for by the *ad hoc* introduction of the average irreversible work,

$$\langle W\rangle = \langle W_{\mathrm{irr}}\rangle + \Delta F.$$

For a closed quantum system, the heat transfer into the system $Q = 0$ and the sole contribution to the change in entropy is the irreversible entropy production, defined as $\Delta S_{\mathrm{irr}} = \beta\langle W_{\mathrm{irr}}\rangle$ [14]. In Ref. [16] it is shown that for an initial Gibbs state $\rho_{\mathrm{G}}(\lambda_0)$ undergoing unitary evolution generated by a time-dependent Hamiltonian $H(\lambda(t))$, the irreversible entropy production is given by the relative entropy of the instantaneous state of the system $\rho(t) = U(t, 0)\rho_{\mathrm{G}}(\lambda_0)U^\dagger(t, 0)$ and a hypothetical Gibbs state at that time, i.e.,

$$\begin{aligned}\Delta S_{\mathrm{irr}} &= S(\rho(t)||\rho_{\mathrm{G}}(\lambda_t)) \\ &= \mathrm{Tr}[\rho(t)\log\rho(t)] - \mathrm{Tr}[\rho(t)\log\rho_{\mathrm{G}}(\lambda(t))].\end{aligned} \tag{5}$$

In the case of a sudden quench, in which the work parameter $\lambda(t)$ is suddenly switched between some initial and final value, we therefore have

$$\Delta S_{\mathrm{irr}} = S(\rho_{\mathrm{G}}(\lambda_0)||\rho_{\mathrm{G}}(\lambda_\tau)). \tag{6}$$

This expression for the irreversible entropy production induced by a sudden quench in a closed quantum system was first noted by Donald in Ref. [17] within a different context.

Transverse quantum Ising model.—We now apply the framework of nonequilibrium statistical mechanics outlined above to the nonequilibrium transformation of a thermal quantum spin chain. In particular, we analyze the sudden quench of the transverse field in the quantum Ising model. For a discussion of this model in the zero temperature limit see Refs. [6,18].

We consider a one-dimensional ring of N spin-1/2 particles that interact with their nearest neighbors via ferromagnetic coupling along the z axis and with an external field applied along the x axis. The Hamiltonian is

$$H(\lambda) := -\sum_{j=1}^{N} \lambda\sigma^x_j + \sigma^z_j\sigma^z_{j+1}, \tag{7}$$

where λ is a dimensionless parameter measuring the strength of the external field with respect to the spin-spin coupling, σ^α_j ($\alpha = x, y, z$) is the spin-1/2 Pauli operator acting at the jth spin and periodic boundary conditions are imposed by requiring that $\sigma^\alpha_{N+1} = \sigma^\alpha_1$. The transverse quantum Ising model possesses a critical point at $\lambda_{\mathrm{c}} = 1$

as the ordering of its ground state changes discontinuously from a paramagnetic ($\lambda > 1$) to a ferromagnetic ($\lambda < 1$) phase. The Hamiltonian Eq. (7) is diagonalized by decomposing the Hilbert space into orthogonal parity subspaces and following the procedure outlined in the Supplemental Material [19]. In this way, considering the positive-parity subspace only, the initial Hamiltonian with $\lambda = \lambda_0$ is written [20]

$$H(\lambda_0) = \sum_{k\in K^+} \epsilon_k(\lambda_0)\left(\gamma_k^\dagger \gamma_k - \frac{1}{2}\right), \tag{8}$$

where γ_k, $\gamma_k^\dagger$ are fermionic creation and annihilation operators labeled by the members of the set $K^+ = \{\pm\pi(2n-1)/N : n = 1, \ldots, N/2\}$ of *positive-parity subspace* pseudomomenta. Proceeding as earlier, the system is prepared in the Gibbs state $\rho_G(\lambda_0) = e^{-\beta H(\lambda_0)}/\mathcal{Z}(\lambda_0)$ with inverse temperature β and associated partition function

$$\mathcal{Z}(\lambda_0) = 2^N \prod_{\substack{k\in K^+ \\ k>0}} \cosh^2\left[\frac{\beta\epsilon_k(\lambda_0)}{2}\right].$$

The protocol constitutes the instantaneous switching of the transverse field to the final value $\lambda = \lambda_\tau$, giving the final Hamiltonian

$$H(\lambda_\tau) = \sum_{k\in K^+} \epsilon(\lambda_\tau)\left(\tilde{\gamma}_k^\dagger \tilde{\gamma}_k - \frac{1}{2}\right). \tag{9}$$

Note that the differing values of the transverse field in Eqs. (8) and (9) require diagonalizing transformations that are quantitatively different. Consequently the postquench fermionic operators $\{\tilde{\gamma}_k\}$ differ from their prequench counterparts $\{\gamma_k\}$, though the allowed values of the psuedomomenta are identical in both cases. In the case of a sudden quench the characteristic function Eq. (2) takes the simplified form

$$\chi_F(u) = \mathrm{Tr}[e^{iuH(\lambda_\tau)} e^{-iuH(\lambda_0)} \rho_G(\lambda_0)]. \tag{10}$$

Using Eqs. (8) and (9), the trace in Eq. (10) is taken over the eigenstates of the initial Hamiltonian $\{|n_k, n_{-k}\rangle\}$ to give

$$\chi_F(u) = \frac{1}{\mathcal{Z}(\lambda_0)} \prod_{\substack{k\in K^+ \\ k>0}} \sum_{n_{\pm k}=0,1} e^{-(iu+\beta)\epsilon_k(\lambda_0)(n_k+n_{-k}-1)} \langle n_k, n_{-k}| e^{iu\epsilon_k(\lambda_\tau)(\tilde{\gamma}_k^\dagger\tilde{\gamma}_k + \tilde{\gamma}_{-k}^\dagger\tilde{\gamma}_{-k}-1)} |n_k, n_{-k}\rangle.$$

The matrix elements can be evaluated explicitly to give an analytic form of the forward characteristic function. Hence,

$$\chi_F(u) = \frac{1}{\mathcal{Z}(\lambda_0)} \prod_{\substack{k\in K^+ \\ k>0}} \{e^{(iu+\beta)\epsilon_k(\lambda_0)}[C_k^-(u,\lambda_\tau) + S_k^+(u,\lambda_\tau)] + e^{-(iu+\beta)\epsilon_k(\lambda_0)}[C_k^+(u,\lambda_\tau) + S_k^-(u,\lambda_\tau)] + 2\}. \tag{11}$$

Here we have introduced the quantities $C_k^\pm(u,\lambda) = \cos^2(\Delta_k/2)e^{\pm iu\epsilon_k(\lambda)}$ and $S_k^\pm(u,\lambda) = \sin^2(\Delta_k/2)e^{\pm iu\epsilon_k(\lambda)}$, where $\Delta_k = \tilde{\phi}_k - \phi_k$ is the difference in the pre- and postquench Bogolyubov angles (see Supplemental Material [19]).

Verification of the fluctuation relations.—The verification of the Tasaki-Crooks relation Eq. (3) requires an expression for the backward characteristic function. This is easily obtained using a procedure similar to that described above for the forward characteristic function Eq. (11) under the mapping $\lambda_0 \leftrightarrow \lambda_\tau \Rightarrow \epsilon_k(\lambda_0) \leftrightarrow \epsilon_k(\lambda_\tau)$, $\Delta_k \to -\Delta_k$. The Tasaki-Crooks relation then follows from $\chi_B(v)$ by introducing the complex parameter $v = -u + i\beta$. Noting that $C_k^\pm(-u+i\beta,\lambda) = C_k^\mp(u,\lambda)e^{\mp\beta\epsilon_k(\lambda)}$ and $S_k^\pm(-u+i\beta,\lambda) = S_k^\mp(u,\lambda)e^{\mp\beta\epsilon_k(\lambda)}$, it is straightforward to show that

$$\chi_B(-u+i\beta) = \frac{1}{\mathcal{Z}(\lambda_\tau)} \prod_{\substack{k\in K^+ \\ k>0}} \{e^{(iu+\beta)\epsilon_k(\lambda_0)}[C_k^-(u,\lambda_\tau) + S_k^+(u,\lambda_\tau)] + e^{-(iu+\beta)\epsilon_k(\lambda_0)}[C_k^+(u,\lambda_\tau) + S_k^-(u,\lambda_\tau)] + 2\}.$$

The ratio of the forward and backward characteristic functions is thus equivalent to the Crooks relation Eq. (3). Further, the Jarzynski equality Eq. (4) follows from the forward characteristic function Eq. (11) by introducing the complex argument $u = i\beta$,

$$\chi_F(i\beta) = \frac{1}{\mathcal{Z}(\lambda_0)} \prod_{\substack{k\in K^+ \\ k>0}} \{2 + 2\cosh[\beta\epsilon_k(\lambda_\tau)]\} = \frac{2^N}{\mathcal{Z}(\lambda_0)} \prod_{\substack{k\in K^+ \\ k>0}} \cosh^2\left[\frac{\beta\epsilon_k(\lambda_\tau)}{2}\right] = \frac{\mathcal{Z}(\lambda_\tau)}{\mathcal{Z}(\lambda_0)}.$$

To our knowledge this is the first analytic demonstration of the fluctuation relations in a non-trivial quantum many-body system incorporating a critical point.

Emergent thermodynamics.—The general form of the forward characteristic function following a sudden quench Eq. (10) admits a simple expression for the average work in terms of its first cumulant, i.e., $\langle W\rangle = d\chi_F/du|_{u=0}$, thus

$$\langle W\rangle = \mathrm{Tr}[H(\lambda_\tau)\rho_G(\lambda_0)] - \mathrm{Tr}[H(\lambda_0)\rho_G(\lambda_0)]. \tag{12}$$

Using the approach presented in the Supplemental Material [19], the evaluation of Eq. (12) leads to the following closed analytic form for the average work done on the spin system

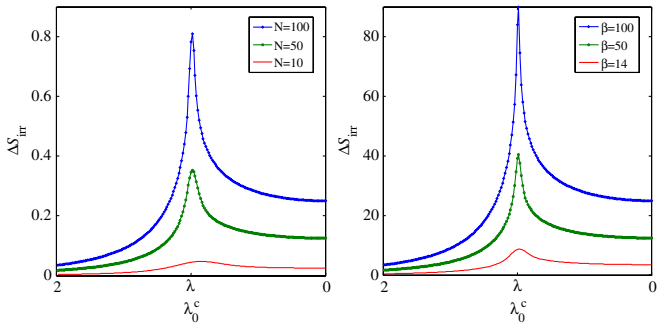


FIG. 1 (color online). Left: The irreversible entropy production for a series of quenches with amplitude $|\lambda_\tau - \lambda_0| = 0.01$ at $\beta = 100$ for several different ring sizes. The initial value of the transverse field λ_0 is shown on the x axis. Right: The irreversible entropy production for the same series of quenches in a ring of $N = 10\,000$ spins at various temperatures.

$$\langle W\rangle = \sum_{\substack{k\in K^+\\ k>0}} [\epsilon_k(\lambda_0) - \epsilon_k(\lambda_\tau)\cos(\Delta_k)]\tanh\left[\frac{\beta\epsilon_k(\lambda_0)}{2}\right]$$
$$= 2(\lambda_0 - \lambda_\tau)\sum_{\substack{k\in K^+\\ k>0}} \cos(\phi_k)\tanh\left[\frac{\beta\epsilon_k(\lambda_0)}{2}\right].$$

This in turn allows the calculation of the irreversible entropy production Eq. (6) for arbitrary temperature, number of spins and quench amplitude;

$$\Delta S_{\rm irr} = \beta\langle W\rangle + \sum_{\substack{k\in K^+\\ k>0}} \ln\frac{\cosh^2[\beta\epsilon_k(\lambda_\tau)/2]}{\cosh^2[\beta\epsilon_k(\lambda_0)/2]}.$$

This quantity and its thermodynamic interpretation encapsulate the physics of the quench problem in a closed critical system in a remarkably simple way. Figure 1 shows the irreversible entropy production due to a series of sudden quenches with amplitude $|\lambda_\tau - \lambda_0| = 0.01$. The left figure shows the quantity for spin chains of several sizes and low temperature $\beta = 100$. The interpretation of the behavior is straightforward: As the size of the system increases the energy gap between the ground and first excited state at the critical point begins to close. Work is performed to drive the system across the critical region and, due to the vanishing energy gap, it becomes increasingly difficult to do so without exciting the system, thereby dissipating work. This leads to increased irreversible entropy production and the emergence of intrinsic irreversibility in the critical region. Alternatively, the irreversible entropy production can be understood in terms of the quantum relative entropy of the instantaneous state and the hypothetical Gibbs state at that time Eq. (5). As noted in Eq. (6), for a sudden quench this coincides with the distance between the Gibbs states of the pre- and postquench Hamiltonians. Near criticality, the equilibrium state changes dramatically for small changes in the transverse field and this is reflected in a sharp increase in irreversible entropy production. This interpretation can be considered as the quantum version of the classical argument presented in Ref. [21]. The asymmetry of the irreversible entropy production away from criticality on either side of the critical point is a consequence of the fact that the relative quench amplitude $|\lambda_\tau - \lambda_0|/\lambda_0$ is larger for $\lambda_0 < 1$.

The figure on the right shows the irreversible entropy production in a chain of $N = 10\,000$ spins at various temperatures. As expected, the signature of quantum criticality decreases at higher temperatures with the emergence of thermal fluctuations. The source of irreversibility is elucidated by manipulating the Tasaki-Crooks fluctuation relation to obtain the expression $\Delta S_{\rm irr} = \int dW P_{\rm F}(W) \times \log[P_{\rm F}(W)/P_{\rm B}(-W)] = \mathcal{K}(P_{\rm F}(W)||P_{\rm B}(-W))$, where $\mathcal{K}$ is the Kullback-Leibler relative entropy, measuring the distance between two probability distributions. Intuitively, this expression attributes the amount of irreversible entropy production to the degree of uncertainty in distinguishing the experimental data contained in the forward and backward work distributions (see, e.g., Ref. [22]). Accordingly, as is evident from Fig. 1, quantum criticality has the effect of setting the thermodynamic arrow of time as the degree of irreversibility grows with decreasing temperature.

As a final remark we note that the forward characteristic function Eq. (2) has a similar form to the Loschmidt echo [23]. This has been shown in previous work to be a good indicator of phase transitions [24] and could be experimentally measured using Ramsey interferometry [25].

R. D. is funded by the EPSRC (UK) ; J. G. acknowledges funding from IRCSET through a Marie Curie International Mobility fellowship; C. C. is supported by the Alexander von Humboldt Foundation; M. P. thanks the EPSRC (UK) a grant under the "New Directions for EPSRC Research Leaders" initiative (EP/G004579/1); V. V. is a fellow of Wolfson College Oxford and is supported by the John Templeton Foundation, the National Research Foundation, the Ministry of Education in Singapore and the Leverhulme Trust (UK). R. D. is grateful to D. K. K. Lee for helpful discussions.

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[20] Here we have abused notation slightly for the sake of brevity. The Hamiltonian in Eq. (8) is the positive-parity contribution to the full Hamiltonian Eq. (7) only. In the main text this is indicated by the sum over the set of positive-parity psuedomomenta K^+. In the Supplemental Material [19], where the full diagonalization of Eq. (7) is discussed, the positive and negative parity contributions to the Hamiltonian are explicitly denoted $H^{\pm}$.
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