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Design for a Room-Temperature Superconductor

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The vision of "room-temperature superconductivity" has appeared intermittently but prominently in the literature since 1964, when W. A. Little and V. L. Ginzburg began working on the *problem of high-temperature superconductivity* around the same time. Since that time the prospects for room-temperature superconductivity have varied from gloom (around 1980) to glee (the years immediately after the discovery of HTS), to wait-and-see (the current feeling). Recent discoveries have clarified old issues, making it possible to construct the blueprint for a viable room-temperature superconductor.

1. PROLOGUE

It is not clear when the mantra "room-temperature superconductivity" first passed the lips of superconductivity researchers, but it has attained some prominence in the literature since Little used it in the title (*Superconductivity at Room Temperature*) of an overview in 1965 [1] of his electronic polarization mechanism proposed for polymeric systems. Ginzburg immediately transitioned this to two-dimensional metal–insulator sandwich materials and generalized the description [2]. Sad to say, these electronic-mediated superconductors are yet to be realized. Uses of the term *room-temperature superconductivity* have ranged from general speculations [3] to glimpses of "glitchite"[4, 5] to editorial coverage of public announcements [6] to preplanning for applications [7]. In the ensuing decades Vitaly Ginzburg has been the most visible and persistent advocate that there is no theoretical justification for pessimism. Ginzburg was elaborating more generally on "high-temperature superconductivity" by [8] 1967 and his optimism has never flagged.

HTS (cuprate high-temperature superconductors) set the standard with $T_c \sim 90$ K in 1987 and rising to ~130 K by the mid-1990s, but there have been no further increases. Since there is no viable theory of the mechanism of HTS, there is no approach that will allow the rational design of new materials with higher T_c in that class. The phonon mechanism however has an accurate microscopic theory that is valid to reasonably strong coupling, and therefore invites the design of materials with higher T_c. The recent and very surprising breakthroughs in phonon-mediated superconductivity can be put to use to provide a plausible recipe for the design of a room-temperature superconductor. This is the purpose of this modest proposal, where a central feature is the emphasis on *control* of the coupling, versus the standard approach of increasing the *brute strength of the coupling*.

2. BACKGROUND

Nearing the end of the 1970s there was pessimism about raising the superconducting transition temperature (T_c) significantly, and there were claims (mostly unpublished) that the maximum T_c was around 30 K. The only superconductivity known at the time (excluding the superfluidity of He [3] which was unlike anything seen in metals) was symmetric (s-wave) pairing mediated by vibrations of the atoms (phonons). The maximum T_c known at the time was 23 K in the A15 system. The maximum T_c had increased by only 6 K in 25 years, and it was not due to increase for several more years (1986, when HTS was announced).

The discovery in 2001 [9] of MgB_2, with $T_c = 40$ K, was stunning not only because of the

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unimaginably high T_c for phonon-mediated superconductivity, but also because it appeared in a completely wrong kind of material according to the accumulated knowledge. This aspect has been dealt with in some detail now [10–14], and the pairing mechanism, character, and strength is well understood. While there has been some effort to apply what has been learned from MgB_2 to find other similar, or even better, superconductors, so far MgB_2 remains in a class by itself. Diamond, when it is heavily doped with B, becomes superconducting [15, 16] with reports as high as 12 K. B-doped diamond has features in common [17–21] with MgB_2 except for the two-dimensionality (2D) of MgB_2's electronic structure. It is this 2D character we deal with here, one important aspect of which has not been emphasized previously. We confine our consideration to ambient pressure; applied pressure could well provide enhancements.

3. STRONG COUPLING THEORY

Migdal–Eliashberg (ME) theory of superconductivity is firmly grounded on the real material level [22] and is one of the impressive successes of condensed matter theory. Stripped to its basics, (phonon coupled) T_c depends on the characteristic frequency Ω of the phonons and on the strength of coupling λ; in the strong coupling regime of interest here the Coulomb pseudopotential loses relevance. The essence of increasing T_c lies in making one or both of these characteristic constants larger while avoiding structural instability. The focus here is on the decomposition of λ [23]

$$\frac{N(E_F)\langle I^2\rangle}{M\langle\omega^2\rangle} = \lambda = \sum_Q \lambda_Q, \tag{1}$$

where the mode-λ for momentum Q is given for circular Fermi surfaces in two dimensions by

$$\lambda_{\vec{Q}} = \frac{2}{\omega_{\vec{Q}} N(0)} d_B^2 \sum_k |\mathcal{M}_{k,k+Q}|^2 \delta(\varepsilon_k)\delta(\varepsilon_k + Q)$$

$$\alpha \ \frac{N(0)}{\omega_Q} d_B^2 |\mathcal{M}|^2 \hat{\xi}(Q), \tag{2}$$

$$\hat{\xi}(Q) = [N(0)]^{-2} \sum_k \delta(\varepsilon_k)\delta(\varepsilon_{k+Q}) = \frac{1}{\eta_Q\sqrt{1-\eta_Q^2}},$$

where $\eta_Q = Q/2k_F$ Here $N(0)$ is the Fermi level ($E_F = 0$) density of states, $\langle I^2\rangle$ is the squared electron-displaced ion matrix element averaged over the Fermi surface, M is the atomic mass, and ω is the characteristic physical phonon frequency. The el–ph matrix element $\mathcal{M}_{k,k+Q}$ involves $I_{k,k+Q}$, M, and ω in the standard way. Here the band degeneracy d_B factor (number of Fermi surfaces) is treated as in MgB_2, where the two σ surfaces are equally important.

In the conventional adiabatic approximation, phonon renormalization is given by the real part of the phonon self-energy at zero frequency

$$\Pi^\sigma(Q) = -2 \sum_{k,n,m} |\mathcal{M}_{k,Q}|^2 \frac{f_{k,n-f_{k+Q,m}}}{\varepsilon_{k+Q,m} - \varepsilon_{k,n}}$$

$$\approx -2|\mathcal{M}|^2 d_B^2 N(0)\hat{\chi}(Q),$$

$$\chi(Q) = 1, \qquad \eta_Q < 1,$$

$$= \left[1 - \sqrt{1-\eta_Q^{-2}}\right], \quad \eta_Q > 1. \tag{3}$$

Both here and above the final expression has been expressed for MgB_2-like systems with cylindrical Fermi surfaces [10, 11, 24–26]. The behavior of this renormalization is pictured in Fig. 1, note specifically the independence of the degree of softening on k_F.

It is the last result (Eq. (3)) that we emphasize here: the phonon renormalization is constant (i.e. controlled) for $Q < 2k_F$, and diminishes quickly for larger Q. For circular Fermi surfaces there is no sharp

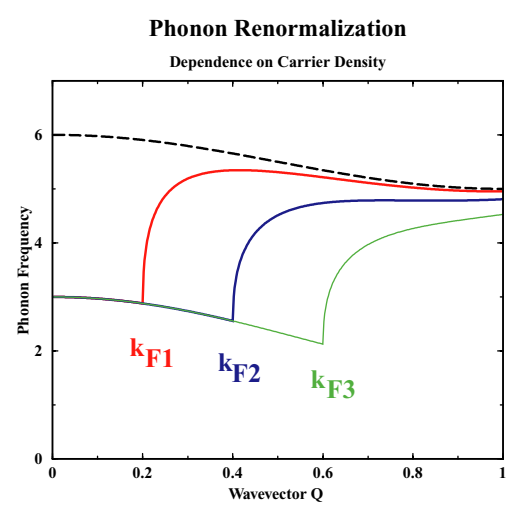

Fig. 1. Illustration of the renormalization of a single optic mode, shown as the *dashed* cosine-like branch, due to carriers with a 2D cylindrical Fermi surface. The downward shift (softening) for $Q < 2k_F$ is proportional to $N(E_F)\langle I^2\rangle$. There are curves for three different densities: lower density, $2k_{F1}$; moderate density, $2k_{F2}$; higher density, $2k_{F3}$. Note in particular that the softening does not depend on the density (k_F).

peak in $\chi(Q)$ at $2k_F$ nor anywhere else. In MgB_2, phonon coupling arises dominantly from $Q < 2k_F$, and only the two bond-stretching branches have the very large matrix elements.

The number of phonon scattering processes from/to the Fermi surface is quantified by the "nesting function" $\hat{\xi}(Q)$ (given here in normalized form whose zone sum is unity). For the 2D circular dispersion relation, it is the simple known quantity in Eq. (3). It has simple integrable divergences at $Q = 0$ and $Q = 2k_F$ which, most importantly, do not result in Q-dependent softening, hence avoiding instability in spite of contributing positively to λ.

This behavior can be contrasted with the vast uncertainty inherent in a general Fermi surface, which has arisen forcefully in recent discoveries. Under pressure elemental Li metal becomes superconducting up to near 20 K as shown by three groups [27–29], in spite of being an s–p metal with a simple Fermi surface [30, 31]. In Fig. 2 $\xi(Q)$ is displayed in three planes [30] in the zone, where extremely sharp structure is apparent. The sharp structure near the K symmetry point leads to a lattice instability (large contribution to $\hat{\chi}(Q)$). The sharp structure occurs in spite of a very simple Cu-like Fermi surface consisting of spheres joined by necks along $\langle 1, 1, 1\rangle$ directions. This example demonstrates why *control* of the Q-dependence of the coupling is essential; λ is not so large [30, 31] for Li at this volume ($\lambda \sim 1.5-3$) yet the lattice has been pushed to instability. This example shows that the overall value of λ is not the indicator of instability of the system, which occurs when some phonon frequency is renormalized (softened) to zero.

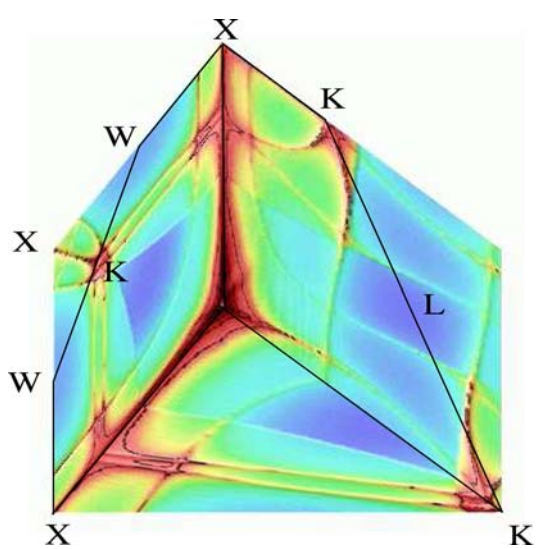

Fig. 2. Intensity plot of the nesting function $\xi(Q)$ for fcc lithium (at 36 GPa) in three planes in the Brillouin zone. The *dark* (red) denotes high intensity, *light* denotes low intensity. $\xi(Q)$ has very sharp structure and high intensities in very localized regions, in spite of the very simple (Cu-like) Fermi surface. A very fine mesh of k-points (2×10^6 in the Brillouin zone) was used to reveal the fine structure.

4. LEARNING FROM RECENT DISCOVERIES

The crucial features to be learned from MgB_2 and Li under pressure follow.

1. High frequency is important; this has long been understood. By beginning from a very stiff unrenormalized lattice, a crystal can withstand a great deal of renormalization to lower frequencies that must accompany strong coupling.
2. Very high mode λ_Q's (up to 20–25 for MgB_2) can arise without instability. MgB_2 appears not to be near any instability, although analysis shows [14] that only ~15–20% stronger coupling would result in instability.
3. The phonon softening in 2D systems due to strong coupling, and the total λ, is independent of carrier concentration (or varies smoothly if the effective mass changes with doping).
4. Impressive results can be obtained from strong coupling to only a fraction of the modes. For MgB_2, $T_c = 40$ K with only 3% of the modes strongly coupled. These modes are the bond-stretch modes (two out of nine branches) with $Q < 2k_F$(12% of the zone).
5. General-shaped Fermi surfaces, even the simple one of Li, can readily lead to lattice instability from a thin surface of soft modes in Q-space. Such instability restricts the achievement of high T_c.
6. Two-dimensional parabolic bands provide *ideal control* of the Q-dependence of coupling strength: phonon renormalization is *constant* for $Q < 2k_F$, not sharply peaking in an unexpected region of the zone as can happen for a Fermi surface of general shape (viz. for Li in Fig. 2).

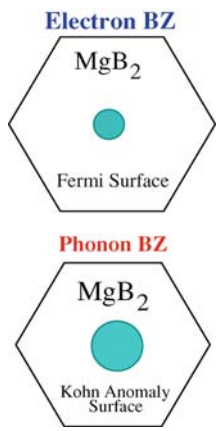

Fig. 3. *Top*: Top view of the hexagonal electron Brillouin zone of MgB_2, with idealized σ-band Fermi surface circle. *Bottom*: The phonon Brillouin zone (same zone, of course), illustrating the simple Kohn anomaly surface with radius (not diameter) $2k_F$.

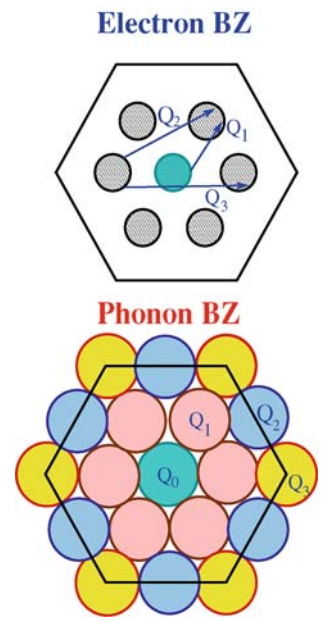

Fig. 4. *Top*: Hexagonal electron Brillouin zone with central Fermi surface circle (an idealization of that of MgB_2) and with six additional circular Fermi surfaces placed at the midpoint of the Γ–K line. *Bottom*: The phonon Brillouin zone, mapping the circular regions $|Q - Q_j| < 2k_F, j = 0, 1, 2, 3$. The figures are drawn for k_F equal to one-eighth of the Γ–K line length, which results in 2D close packing of the circles of diameter $4k_F$. The Kohn circles at the edge have been pictured extending into the neighboring zones to facilitate comparison with the top panel.

5. PUTTING IT ALL INTO A DESIGN

5.1. What We Have

The superconducting T_c of MgB_2 is remarkable, and arises from the extreme strong coupling of 3% of its phonons. The electron–phonon deformation potential $\langle I^2 \rangle^{1/2}$ is very large for the bondstretch modes, and MgB_2 gains a factor $d_B^2 = 4$ from having two Fermi surfaces. Figure 3 illustrates (1) the σ-band Fermi surfaces, idealized to identical circular surfaces, and (2) the Kohn-anomaly region of renormalized phonons $Q < 2k_F$. In MgB_2 this "Kohn surface" encloses only 12% of the zone. Previous analysis [14] has shown that pushing these phonons further, by either increasing the bare coupling strength $N(E_F)\langle I^2 \rangle$ or varying the lattice stiffness (bare phonon frequency) separately, could increase T_c by perhaps 20% but then would drive the material to a lattice instability. It is fairly obvious that if one increases both proportionately, then one gains by enhancing the characteristic frequency while keeping λ constant. This is the metallic hydrogen scenario that was discussed originally 40 years ago [32].

5.2. What We Need

There is however the equally obvious approach: introduce more phonons into the coupling. Here the *control* over the strength of the coupling, for *specific momenta* [that is, λ_Q, or more specifically $\chi(Q)$] becomes essential. The requirement is to renormalize frequencies in other parts of the zone *without further softening* the ones that are already very strongly renormalized, which would lead to lattice instability. Two-dimensional circularly symmetric dispersion relations provide that control, as demonstrated by the equations above. Adding an additional circular Fermi surface centered at Q_1 gives another region of renormalized phonons, and contributions λ_Q to λ, of radius $2k_F$ centered at Q_1.

Let us skip directly to the optimal case, illustrated in Fig. 4. By adding to the MgB_2 zone-centered surface another spherical Fermi surface half-way along the Γ–K line, with radius 1/8 of the length of the Γ–K line, one obtains three new spanning vectors Q_1, Q_2, Q_3, and their symmetry partners that produces an array of close-packed Kohn surfaces of radius $2k_F$ within which coupling is strong. Given the close-packing fraction in 2D, $\pi/2\sqrt{3} = 0.907$, this arrangement manages to utilize 90% of the zone for strongly coupled phonons, an increase in fraction of zone used, compared to MgB_2 (12%), by a factor of 7.5.

This extension from MgB_2 is not yet optimum, because MgB_2 uses only 2/9 of its branches. Optimally, every branch would be drafted into service in strong coupling, giving another factor of 4.5, or a total enhancement of ~30–35. The strongly coupled modes in MgB_2 have mode-λ_Q's of mean value 20–25 (calculations so far have not been precise enough to pin this down). Let us not be pessimistic, and therefore use $\bar{\lambda}_Q = 25$; this value is consistent with the value of λ from the strongly coupled modes divided by 3%, i.e. $0.7/0.03 \sim 23$. Then with 90% participation of the phonons $\lambda = 25 \times 0.90 = 22.5$. Using the Allen–Dynes equation [33] to account properly for the strong-coupling limit that is being approached, and using the MgB_2 frequency of 60 meV, one obtains $T_c = 430$ K. The strong coupling limit [34] of the ratio $2\Delta/k_B T_c$ is 13, so we can estimate the gap of such a superconductor to be $2\Delta \sim 12 k_B T_c \sim 0.4$ eV. This will be an interesting superconductor indeed.

5.3. Where to Look

Whereas the architectural design of a room temperature superconductor provided here is straightforward, the structural engineering necessary to implement this vision will require creativity and knowledge of materials. Where does one look?

5.3.1 More Fermi Surfaces

Figure 4 gives an idea of a set of Fermi surfaces that could be promising. This pattern is very much like that of Na_xCoO_2, although its $T_c = 4.5$ K, and even that not necessarily from phonons, is not a good example of strong coupling enhanced by Fermi surface arrangement. (The zone-centered Fermi surface in Na_xCoO_2 is much larger than the others.) The encouraging feature to be emphasized here is that this example shows that the desirable arrangement of Fig. 4 is nothing unusual. Not only are the Fermi surfaces very near the midpoint of the Γ–K line, but they are nearly circular although not enforced by symmetry.

A more provocative example is that of the layered, electron doped system Li_xMNCl, which has up to $T_c = 15$ K for M = Zr, and $T_c = 26$ K for M=Hf. For $0 < x < 0.4$, which probably includes the accessible concentrations, this system has very nearly circular K-centered Fermi surfaces whose nesting possibilities have been noted [36, 37]. There are surfaces at two inequivalent points K, resulting in Kohn regions centered at the zone center (degeneracy two) and (because $K \to K$ scattering involves momentum transfer K in the hexagonal zone) at each of the pair of points K (also degeneracy two). The figure of Kohn surfaces would look like Fig. 4 with circles centered at Q_1 and Q_2 points missing. Indeed, Heid and Bohnen [37] calculate phonon softening around K and the zone center, but alas they find that the calculated coupling strength comes well short of accounting for $T_c = 15$ K in Li_xZrNCl (not to mention the question of $T_c = 26$ K in Li_xHfNCl). The superconductivity in this system remains unexplained, but the placement of its 2D circular Fermi surfaces illustrates the first step in pulling more phonons into the coupling.

5.3.2 More Phonon Branches

While the electronic system we seek is 2D in character, we also seek (strong) coupling to phonons of arbitrary momentum and polarization. MgB_2 is a bad example here, since the strong bonding lies solely within the layer; the $\hat{z}$-axis modes are hardly coupled. A lattice with strong bonds with substantial component perpendicular to the layers have a better likelihood of coupling to bond stretch modes. From this point of view the Li_xZrNCl system seems to be a step in the right direction, as it has Zr–N bonds both within the layer and perpendicular to it. Heid and Bohnen [37] found moderate coupling both to two stiff modes (~65 meV, primarily N) and to two softer modes (~25 meV). These modes are however polarized in-plane; the perpendicular Zr–N modes do not couple to the 2D electronic system. Creativity will be required to find how to involve a larger fraction of modes in the coupling.

6. REMAINING ISSUES

Since there may be people who are truly interested in this topic of room-temperature superconductivity, the basic premises and concepts should be made as clear and precise as possible ("truth in advertising"). The following issues should be mentioned:

1. The use of the term *optimal* as used above was disingenuous and incorrect, and that discussion as it stands is unduly pessimistic. Close-packing of $4k_F$-diameter Kohn circular surfaces does

indeed use the area of the zone efficiently (although mathematicians or engineers would fill the holes with smaller circles, and then again and again ad infinitum, thereby using 100% of the area). However, maximizing the area is *not* the objective. The objective is to maximize T_c or to simplify slightly for now, to maximize λ. Phase space in 2D leads to the non-intuitive result that integration of λ_Q over a Kohn region of diameter $4k_F$ is independent of k_F, as long as the ME theory we are applying holds. The objective then is to maximize the number of Kohn regions. Since there are likely to be different values of $N(0)\langle I^2\rangle$ and ω for the different regions, it will be something like the quantity

$$\sum_j^{\mathcal{N}_K} \frac{[N(0)\langle I^2\rangle]_j}{\omega_j}, \tag{4}$$

that needs maximizing, where $\mathcal{N}_k$ is the (variable) number of Kohn regions.

2. Care must be taken to keep the Kohn regions from overlapping if the combined renormalization of phonons will be so strong as to drive instability. Also, the band degeneracy factor d_B seems to be extremely helpful, but must be watched. (In Eq. (4) there would be some factor related to d_B of identical terms.) For example, in Fig. 4 each of the Fermi surfaces contributes (via intrasurface scattering) to the coupling strength and accompanying phonon softening inside the Kohn region at $Q_0 = 0$, a factor of 12 in this case. A good strategy would be to have matrix elements be larger for Q_1, Q_2, Q_3, which have smaller degeneracy factors, than for Q_0 with its large multiplier, thereby crafting strong coupling while avoiding the $Q = Q_0$ instability.
3. The validity of the theory bears reconsideration. It is safe to say that if $\lambda_Q(\omega_Q/E_F) \ll 1$ for every phonon Q, then ME (second order perturbation) theory is safe. If this inequality is not satisfied for a small fraction of the coupling strength, corrections are probably minor. However, for the typical strongly coupled phonon in MgB_2,

$$\lambda_Q \frac{\omega_Q}{E_F} \sim 25 \frac{60\,\text{meV}}{400\,\text{meV}} \sim 4. \tag{5}$$

The condition of validity is violated badly for *every important phonon*, making ME theory in MgB_2 unjustified as pointed out earlier [38–40]. Nevertheless, its predictions seem to be reasonable for MgB_2, so it is reasonable for us to extrapolate the theory to include more phonons with similar strength of coupling.
4. It was noted above that for a frequency $\omega \sim 60$ meV as in MgB_2, $\lambda \sim 20$ is required to reach the vicinity of room-temperature. While there have been many papers addressing the very strong regime and resulting polarons and bipolarons, we are not aware of any that address seriously such coupling in a degenerate electron system. There is a general expectation that the electron system becomes unstable, but unstable to what is unclear; a degenerate dense gas of polarons (of the order of one per atom) does not seem like a clear concept. (If the instability occurs only below T_c, it may not control or limit the pairing at high temperature.) The description of such a system is still unknown; while MgB_2 has a finite concentration (3%) of *extremely* strongly coupled phonons, the net value of λ is less than unity. Following the materials design proposed here will lead to study of a new materials regime as well as higher T_c.

7. PROSPECTS FOR SUCCESS

A blueprint for the design of a room-temperature superconductor has been provided here. The essence is this: very strong Q-dependent coupling in a *controlled* fashion is possible, and one follows the path toward getting as much as one can out of both the electronic and the phononic systems. Two-dimensional electronic structures with circular Fermi surfaces give an unsurpassed level of control of the Q-dependence, which if uncontrolled can and does lead to structural instabilities even at moderate total coupling strength. Stiff lattices are important, as is getting as many of the branches as possible involved in coupling.

On the one hand, MgB_2, impressive as it is, seems to be doing a poor job in most respects of making use of the available phase space. MgB_2 uses only 12% of all the possible phonon momenta, and only 2/9 of its phonon branches, netting only 3% of phonons involved in coupling. MgB_2 excels at producing extremely large electron-displaced ion matrix elements, and its 2D phase space keeps the extremely large coupling (to those 3%) firmly under control. All things considered, it seems reasonable to expect that

materials exist, or can be made, that will improve on MgB_2's current record.

There is no promise here, nor even expectation, that such improvement will be easy. Although one can employ tight-binding models to suggest crystal structures and interatomic interactions that will place band extrema in the desired positions in the zone, synthesizing the corresponding material is more uncertain. We work with discrete nuclear charges, so this is a Diophantine problem rather than a continuous one, and bonding properties can change rapidly from atom to atom. In addition, incremental improvements lead to even more incremental payoffs. The behavior [33] of $T_c(\lambda)\alpha\sqrt{\lambda}$ in the strong-coupling regime, while monotonically increasing, provides a law of diminishing returns: doubling T_c requires quadrupling λ, a sobering prospect. Finally, it should be re-emphasized that no realistic theory of the degenerate electronic system in the presence of phonon coupling in the regime $\lambda > 5$ (say) exists, but this is another, perhaps better, physical reason to push to stronger coupling systems. And think of it-would not it be really great to carry around a spool of superconducting D_2E_3Z wire in your pocket?

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